DIRAC NOTATION

BASIC OBJECTS

- Dirac notation is a new notation, not a new theory. It's a new way of writing vectors, instead of the familiar $\vec{\alpha}$. We introduce it in QM because it makes vector computations much simpler and much more natural. Yet it doesn't have conceptually anything more than the usual $\vec{\alpha}$ notation.

- What is conceptually different in QM though, is that we use both finite- and infinite-dimensional vector spaces (instead of the familiar 3-dimensional $\mathbb{R}^3$), and moreover in the infinite case we can have both countable (= discrete = enumerated by integers) bases and uncountable (= continuous = enumerated by real numbers) bases, and vector spaces are over complex numbers (not real!).
- We won't define here the basic objects we deal with in QM (though linear algebra provides of course all these definitions); instead, you should gain intuition of what they are by understanding them in the familiar case of the Euclidian vector space $\mathbb{C}^N$; and you must remember what they are:

BASIC OBJECT	NAME	WHAT KIND OF OBJECT IS IT?	WHAT IT CORRESPONDS TO IN THE SPECIAL CASE OF EUCLIDIAN $\mathbb{C}^N$
$\lvert\alpha\rangle$	ket	vector	$\begin{pmatrix}\alpha_1\\ \alpha_2\\ \vdots\\ \alpha_N\end{pmatrix}$ (column vector, i.e. N×1 matrix)
$\langle\alpha\rvert$	bra	vector	$(\alpha_1^* \; \alpha_2^* \dots \alpha_N^*)$ (row vector, i.e. 1×N matrix)
$\langle\alpha\vert\beta\rangle$	inner product	complex number	$\underbrace{(\alpha_1^* \; \alpha_2^* \dots \alpha_N^*)}_{1\times N}\underbrace{\begin{pmatrix}\beta_1\\ \beta_2\\ \vdots\\ \beta_N\end{pmatrix}}_{N\times 1} = \underbrace{\alpha_1^*\beta_1+\alpha_2^*\beta_2+\dots+\alpha_N^*\beta_N}_{1\times 1}$
$\lvert\alpha\rangle\langle\beta\rvert$	outer product	linear operator	$\underbrace{\begin{pmatrix}\alpha_1\\ \alpha_2\\ \vdots\\ \alpha_N\end{pmatrix}}_{N\times 1}\underbrace{(\beta_1^* \; \beta_2^* \dots \beta_N^*)}_{1\times N} = \underbrace{\begin{pmatrix}\alpha_1\beta_1^* & \alpha_1\beta_2^* & \dots & \alpha_1\beta_N^*\\ \alpha_2\beta_1^* & \alpha_2\beta_2^* & \dots & \alpha_2\beta_N^*\\ \vdots & \vdots & \ddots & \vdots\\ \alpha_N\beta_1^* & \alpha_N\beta_2^* & \dots & \alpha_N\beta_N^*\end{pmatrix}}_{N\times N}$

- Note about operators: We see above that by analogy with the $\mathbb{C}^N$ case, the object $|\alpha\rangle\langle\beta|$ is an operator – for $\mathbb{C}^N$ it's an $N \times N$ matrix. There's also another way to understand it, which moreover highlights a very important advantage of Dirac notation:

An operator is something that acting on a ket produces another ket. So let's act with $|\alpha\rangle\langle\beta|$ on a ket $|\gamma\rangle$ and see if indeed we obtain a ket:

$$\overbrace{|\alpha\rangle\langle\beta|}^{?}\overbrace{|\gamma\rangle}^{\text{KET}}. \quad \longleftarrow \text{"OLD VIEWPOINT"}$$

$$\underbrace{|\alpha\rangle}_{\text{KET}}\underbrace{\langle\beta|\gamma\rangle}_{\text{NUMBER}}. \quad \longleftarrow \text{"NEW VIEWPOINT"}$$

IT'S EASY AND NATURAL TO VIEW IN DIFFERENT WAYS OBJECTS WRITTEN IN DIRAC NOTATION (AND YOU <u>MUST</u> KNOW THE TABLE ON P. 1 TO DO THIS!)

Thanks to Dirac notation, we can understand $|\alpha\rangle\langle\beta|\gamma\rangle$ <u>in two ways</u>: <u>either</u> as the object $|\alpha\rangle\langle\beta|$ (which we want to find out what it is) times the ket $|\gamma\rangle$, <u>or</u> as the ket $|\alpha\rangle$ times the complex number $\langle\beta|\gamma\rangle$. <u>This simple possibility of viewing in different ways objects written in Dirac notation, is one of its greatest advantages.</u> So now we see that the object $|\alpha\rangle\langle\beta|$ acting on the ket $|\gamma\rangle$ produces the ket $|\alpha\rangle$ times the complex number $\langle\beta|\gamma\rangle$, i.e. indeed another ket (a vector times a number is a vector), and so $|\alpha\rangle\langle\beta|$ must be an operator:

$$\overbrace{|\alpha\rangle\langle\beta|}^{\text{OPERATOR}}\overbrace{|\gamma\rangle}^{\text{KET}}. \quad \longleftarrow \text{"OLD VIEWPOINT"}$$

$$\underbrace{|\alpha\rangle}_{\text{KET}}\underbrace{\langle\beta|\gamma\rangle}_{\text{NUMBER}}. \quad \longleftarrow \text{"NEW VIEWPOINT"}$$

- The symbol "α" above in $|\alpha\rangle$ or $\langle\alpha|$ is <u>any description of the ket/bra we find useful to apply</u>; this is another advantage of Dirac notation, absent in the $\vec{\alpha}$ notation. For example, it can be even something like:

$$\boxed{|\text{living cat}\rangle}$$

(from the Schrödinger's cat experiment), allowing to write funny-looking things like $|\text{cat}\rangle = \frac{1}{\sqrt{2}}(|\text{living cat}\rangle + |\text{dead cat}\rangle)$.

- You may ask what is <u>a relationship between kets and bras.</u> Though we could state it precisely, here let's just mention that a linear combination of kets, $a|\alpha\rangle + b|\beta\rangle$, with $a, b \in \mathbb{C}$, corresponds to the bra:

$$\boxed{a|\alpha\rangle + b|\beta\rangle \quad \longleftrightarrow \quad a^*\langle\alpha| + b^*\langle\beta|.}$$

REPRESENTATION OF A KET IN AN ORTHONORMAL BASIS

- Vectors and operators are abstract mathematical objects, and they are meaningful even before any basis in the vector space is chosen; their existence is prior to choosing a basis.

  But for practical purposes, it's often useful to choose a particular basis, and consider the representation of a given vector or operator in this basis. It's clear that representation has a meaning only after a basis is chosen, and that representation depends on a basis (i.e. will be different if we change the basis).

- We are already acquainted with finite-dimensional vector spaces (say, N-dimensional), in which a basis consists of N vectors:

$$\boxed{\{|1\rangle, |2\rangle, \ldots, |N\rangle\} \equiv \{|i\rangle : i = 1, 2, \ldots, N\}.}$$

It doesn't take much conceptual effort to generalize this to countably-dimensional vector spaces, i.e. in which a basis consists of infinitely many but still countably many vectors (i.e. they can be enumerated by integers):

$$\boxed{\{|1\rangle, |2\rangle, \ldots\} \equiv \{|i\rangle : i = 1, 2, \ldots\}.}$$

But what is most often in QM is uncountably-dimensional vector spaces, i.e. in which a basis consists of infinitely and uncountably many vectors (i.e. they can't be enumerated by integers, they need to be enumerated by real numbers), like:

$$\boxed{\{|x\rangle : x \in \mathbb{R}\}.}$$

We'll see below that all computations in the uncountable case are exactly the same as in the countable case, provided we change summation to integration and Kronecker delta to Dirac delta. So don't be scared by the continuous case!

(Don't confuse the symbol "x" here with the position in QM! $\{|x\rangle : x \in \mathbb{R}\}$ is not the position basis, but as for now it's an arbitrary continuous basis.)

Later we'll call countable bases – "discrete", and uncountable – "continuous".

- Let's remind what Kronecker delta and Dirac delta are.

The first one is very simple: It's defined for two integers i, j as:

$$\boxed{\delta_{ij} \equiv \begin{cases} 1, & \text{if} \quad i=j, \\ 0, & \text{if} \quad i \neq j. \end{cases}}$$

For example: $\delta_{5,5} = 1$, $\delta_{8,3} = 0$. It's often used inside sums, and have this basic property:

$$\boxed{\sum_i f_i \delta_{ij} = f_j,}$$

for any sequence $f_1, f_2, \ldots$ Proof:

$$\sum_i f_i \delta_{ij} = f_1 \underbrace{\delta_{1j}}_{0} + f_2 \underbrace{\delta_{2j}}_{0} + \ldots + f_{j-1} \underbrace{\delta_{j-1,j}}_{0} + f_j \underbrace{\delta_{jj}}_{1} + f_{j+1} \underbrace{\delta_{j+1,j}}_{0} + \ldots =$$

(ONLY THIS TERM IS NON-ZERO)

$$= f_j.$$

So Kronecker delta δ_{ij} used inside a sum over i kills all the terms except the one for which $i=j$.

The second delta is conceptually more involved but practically is equally simple. It's defined for two real numbers x, x', but we won't really give its definition (it's not even a usual function but so-called distribution). Instead, we state that it's often used inside integrals, and have this basic property:

$$\boxed{\int_{-\infty}^{+\infty} dx\, f(x)\, \delta(x-x') = f(x'),}$$

i.e. it kills all the integration except the single point for which $x=x'$. This property is practically everything you need to know about Dirac delta.

You can practice using this formula by proving a few properties of Dirac delta, like for example:

$$\boxed{\begin{array}{lll} (1) & \delta(ax) = \frac{1}{|a|}\delta(x), & a \in \mathbb{R}\setminus\{0\}, \\ (2) & \delta(x^2-a^2) = \frac{\delta(x-a)+\delta(x+a)}{2|a|}, & a \in \mathbb{R}\setminus\{0\}, \\ (3) & \delta(g(x)) = \sum_i \frac{1}{|g'(x_i)|}\delta(x-x_i), & \text{where } x_i \text{ are zeros of } g,\ g(x_i)=0, \\ & & \text{provided } g'(x_i)\neq 0. \end{array}}$$

(Formulas (1) and (2) are special cases of the general formula (3).)
Proof of (1) is as follows:

$$\int_{-\infty}^{+\infty} dx\, f(x)\,\delta(ax) = \{ y \equiv ax \} = \frac{1}{|a|}\int_{-\infty}^{+\infty} dy\, f\left(\frac{y}{a}\right)\delta(y) = \frac{1}{|a|} f(0) = \frac{1}{|a|}\int_{-\infty}^{+\infty} dx\, f(x)\,\delta(x),$$

and similarly for (2) and (3), by an appropriate change of variables $x \to y$.

- The most useful type of basis is an orthonormal basis. A discrete basis $\{|i\rangle : i = 1, 2, \ldots\}$ is called "orthonormal" if:

$$\boxed{\langle i|j\rangle = \delta_{ij}.}$$

A continuous basis $\{|x\rangle : x \in \mathbb{R}\}$ is called "orthonormal" if:

$$\boxed{\langle x|x'\rangle = \delta(x - x').}$$

- Let's pick now an arbitrary ket $|\psi\rangle$ in our vector space, and let's choose a discrete orthonormal basis $\{|i\rangle : i = 1, 2, \ldots, N\}$; let's find the representation of the ket $|\psi\rangle$ in the basis $\{|i\rangle : i = 1, 2, \ldots, N\}$ (N can be $N = +\infty$):

$$|\psi\rangle = \sum_{i=1}^{N} \psi_i |i\rangle;$$

it's a linear combination (=superposition) of the basis vectors $|i\rangle$ with some complex coefficients ψ_i, and the set of this coefficients, which can be written as a column vector:

$$\begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_N \end{pmatrix} \equiv [\psi]$$

is called "representation of $|\psi\rangle$ in the basis $\{|i\rangle : i = 1, 2, \ldots, N\}$".

Now we can compute the representation coefficients as follows: We multiply the decomposition $|\psi\rangle = \sum_{i=1}^{N} \psi_i |i\rangle$ by $\langle j|$ from the left, for some fixed j:

$$\langle j|\psi\rangle = \underbrace{\langle j|\left(\sum_{i=1}^{N} \psi_i |i\rangle\right)}_{\text{(LINEARITY)}} = \sum_{i=1}^{N} \psi_i \underbrace{\langle j|i\rangle}_{=\delta_{ji}\ \text{(ORTHONORMALITY)}} = \psi_j,$$

i.e.:

$$\boxed{|\psi\rangle = \sum_{i=1}^{N} \psi_i \underbrace{|i\rangle}_{\text{KET}}, \qquad \psi_i = \underbrace{\langle i|\psi\rangle}_{\text{NUMBER}},}$$

or for short:

$$\boxed{|\psi\rangle = \sum_{i=1}^{N} \underbrace{|i\rangle}_{\text{KET}} \underbrace{\langle i|\psi\rangle}_{\text{NUMBER}}.}$$

Let's now investigate what happens in the continuous case. Let's pick any ket $|\psi\rangle$, and choose an orthonormal continuous basis $\{|x\rangle : x \in \mathbb{R}\}$. The computation is completely parallel: We decompose:

$$|\psi\rangle = \int_{-\infty}^{+\infty} dx\, \psi(x)|x\rangle$$

(it's a continuous basis, so instead of summation we have integration), multiply it from the left by $\langle x'|$, for some fixed x':

$$\langle x'|\psi\rangle = \langle x'| \underbrace{\int_{-\infty}^{+\infty} dx\, \psi(x)|x\rangle}_{\text{(LINEARITY)}} = \int_{-\infty}^{+\infty} dx\, \psi(x) \underbrace{\langle x'|x\rangle}_{\overset{\shortparallel}{\delta(x'-x)} \ \text{(ORTHONORMALITY)}} = \psi(x'),$$

which gives:

$$\boxed{|\psi\rangle = \int_{-\infty}^{+\infty} dx\, \psi(x) \underbrace{|x\rangle}_{\text{KET}}, \qquad \psi(x) = \underbrace{\langle x|\psi\rangle}_{\text{NUMBER}},}$$

or for short:

$$\boxed{|\psi\rangle = \int_{-\infty}^{+\infty} dx\, \underbrace{|x\rangle}_{\text{KET}} \underbrace{\langle x|\psi\rangle}_{\text{NUMBER}}.}$$

- The above computation reveals another crucial advantage of Dirac notation. Notice that we can use its "different viewpoints" property as follows:

$$|\psi\rangle = \underbrace{\sum_{i=1}^{N} \overbrace{|i\rangle}^{\text{KET}}}_{\text{OPERATOR}} \overbrace{\underbrace{\langle i|\psi\rangle}_{\text{KET}}}^{\text{NUMBER}} \qquad\qquad |\psi\rangle = \underbrace{\int_{-\infty}^{+\infty} dx\, \overbrace{|x\rangle}^{\text{KET}}}_{\text{OPERATOR}} \overbrace{\underbrace{\langle x|\psi\rangle}_{\text{KET}}}^{\text{NUMBER}},$$

i.e. what we understood as the ket $|i\rangle$ times the number $\langle i|\psi\rangle$, summed over i, can be also understood as the operator $\sum_{i=1}^{N} |i\rangle\langle i|$ times the ket $|\psi\rangle$ (and similarly in the continuous case, the ket $|x\rangle$ times the number $\langle x|\psi\rangle$, integrated over x, is the same as the operator $\int_{-\infty}^{+\infty} dx\,|x\rangle\langle x|$ times the ket $|\psi\rangle$). Hence for any ket $|\psi\rangle$, if we act on it with this operator $\sum_{i=1}^{N} |i\rangle\langle i|$ (discrete case) / $\int_{-\infty}^{+\infty} dx\,|x\rangle\langle x|$ (continuous case), we obtain the same ket $|\psi\rangle$, which means it's <u>the identity operator</u>:

$$\boxed{\sum_{i=1}^{N} |i\rangle\langle i| = \hat{1},}$$

$$\boxed{\int_{-\infty}^{+\infty} dx\,|x\rangle\langle x| = \hat{1}.}$$

This is known as <u>the completeness relation</u> or <u>decomposition of identity</u>, and is another reason why we use Dirac notation – we'll see that using this formula significantly shortens calculations; you <u>must</u> know it by heart!

For example, you don't need to learn by heart how the representation of a ket $|\psi\rangle$ in an orthonormal basis $\{|i\rangle : i = 1, 2, .., N\}$ (discrete case) / $\{|x\rangle : x \in \mathbb{R}\}$ (continuous case) looks like. It's enough you remember that to obtain it, you insert the identity operator $\hat{1}$, built out of the basis vectors, before $|\psi\rangle$:

$$|\psi\rangle = \overbrace{\sum_{i=1}^{N} \underbrace{|i\rangle}_{\text{KET}} \langle i|}^{\text{OPERATOR}} \overbrace{\underbrace{|\psi\rangle}_{}}^{\text{KET}}$$

$$|\psi\rangle = \sum_{i=1}^{N} \underbrace{|i\rangle}_{\text{KET}} \underbrace{\langle i|\psi\rangle}_{\text{NUMBER}}, \qquad \uparrow\; \hat{1} = \sum_{i=1}^{N} |i\rangle\langle i|$$

$$|\psi\rangle = \overbrace{\int_{-\infty}^{+\infty} dx\,|x\rangle\langle x|}^{\text{OPERATOR}} \overbrace{|\psi\rangle}^{\text{KET}} = \int_{-\infty}^{+\infty} dx\,\underbrace{|x\rangle}_{\text{KET}} \underbrace{\langle x|\psi\rangle}_{\text{NUMBER}}, \qquad \uparrow\; \hat{1} = \int_{-\infty}^{+\infty} dx\,|x\rangle\langle x|$$

REPRESENTATION OF AN OPERATOR IN AN ORTHONORMAL BASIS

- Now instead of an arbitrary ket $|\psi\rangle$, let's consider an arbitrary linear operator $\hat{A}$, and let's choose an orthonormal basis $\{|i\rangle : i = 1, 2, .., N\}$ (discrete case) / $\{|x\rangle : x \in \mathbb{R}\}$ (continuous case).

A ket $|\psi\rangle$ is represented in this basis by <u>a column of numbers</u> $\begin{pmatrix}\psi_1\\ \psi_2\\ \vdots\end{pmatrix}$, where $\psi_i = \langle i|\psi\rangle$ (discrete case) / <u>a function $\psi(x)$</u>, where $\psi(x) = \langle x|\psi\rangle$ (continuous case), such that $|\psi\rangle = \sum_{i=1}^{N} |i\rangle\,\psi_i$ (discrete case) / $|\psi\rangle = \int_{-\infty}^{+\infty} dx\,|x\rangle\,\psi(x)$ (continuous case). Similarly, an operator $\hat{A}$ is in this basis represented by <u>an $N \times N$ matrix</u> in the discrete case:

$$\begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1N} \\ A_{21} & A_{22} & \cdots & A_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ A_{N1} & A_{N2} & \cdots & A_{NN} \end{pmatrix} \equiv [A],$$

or by a function of two arguments in the continuous case:

$$A(x, x'),$$

such that:

$$\boxed{\hat{A} = \sum_{i=1}^{N} \sum_{j=1}^{N} \underbrace{A_{ij}}_{\text{NUMBER}} \underbrace{|i\rangle\langle j|}_{\text{OPERATOR}},}$$

$$\boxed{\hat{A} = \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dx' \underbrace{A(x, x')}_{\text{NUMBER}} \underbrace{|x\rangle\langle x'|}_{\text{OPERATOR}}.}$$

It's very easy to find expressions for A_{ij} (discrete case) / $A(x, x')$ (continuous case) using our "insertion of identity" trick:

$$\hat{A} = \sum_{i=1}^{N} \sum_{j=1}^{N} \overbrace{|i\rangle\langle i|}^{\text{OPERATOR}} \overbrace{\hat{A}}^{\text{OPER.}} \overbrace{|j\rangle\langle j|}^{\text{OPERATOR}} \quad \Rightarrow \quad A_{ij} = \langle i|\hat{A}|j\rangle,$$

$$\hat{A} = \sum_{i=1}^{N} \sum_{j=1}^{N} \underbrace{|i\rangle}_{\text{KET}} \underbrace{\langle i|\hat{A}|j\rangle}_{\text{NUMBER}} \underbrace{\langle j|}_{\text{BRA}}$$

$$\hat{1} = \sum_{j=1}^{N} |j\rangle\langle j|$$

$$\hat{1} = \sum_{i=1}^{N} |i\rangle\langle i|$$

and similarly in the continuous case. Hence:

$$\boxed{A_{ij} = \langle i|\hat{A}|j\rangle,}$$

$$\boxed{A(x, x') = \langle x|\hat{A}|x'\rangle.}$$

This is <u>the representation of the operator $\hat{A}$ in the basis $\{|i\rangle : i = 1, 2, \ldots, N\}$ (discrete case) / $\{|x\rangle : x \in \mathbb{R}\}$ (continuous case).</u>

- Example: Problem 2.1. Here we have a 2-dimensional vector space ($N=2$), and we choose an orthonormal basis $\{|1\rangle, |2\rangle\}$. We're given an operator $\hat{A} = 2|1\rangle\langle 1| + 3|2\rangle\langle 2| + |1\rangle\langle 2| + |2\rangle\langle 1|$, and we want to write its representation in the basis $\{|1\rangle, |2\rangle\}$, $[A]$. We see that A_{ij} is precisely the number that stands by $|i\rangle\langle j|$, hence: $A_{11} = 2$, $A_{22} = 3$, $A_{12} = 1$, $A_{21} = 1$, or for short: $[A] = \begin{pmatrix} 2 & 1 \\ 1 & 3 \end{pmatrix}$.

WHY REPRESENTATIONS?

- Let's collect what we've done. We consider a ket $|\psi\rangle$ and an operator $\hat{A}$. We choose an orthonormal basis $\{|i\rangle : i = 1, 2, .., N\}$ (discrete case) / $\{|x\rangle : x \in \mathbb{R}\}$ (continuous case).

  Representation of the ket $|\psi\rangle$ in this basis is a column of N complex numbers $\begin{pmatrix}\psi_1\\ \psi_2\\ \vdots\\ \psi_N\end{pmatrix}$ (discrete case) / a complex function $\psi(x)$ (continuous case), such that:

$$\boxed{|\psi\rangle = \sum_{i=1}^{N} |i\rangle \psi_i, \qquad \psi_i = \langle i|\psi\rangle,}$$

$$\boxed{|\psi\rangle = \int_{-\infty}^{+\infty} dx\, |x\rangle \psi(x), \qquad \psi(x) = \langle x|\psi\rangle.}$$

  Representation of the operator $\hat{A}$ in this basis is a complex $N\times N$ matrix $[A]$ (discrete case) / a complex function with two arguments $A(x, x')$ (continuous case), such that:

$$\boxed{\hat{A} = \sum_{i=1}^{N} \sum_{j=1}^{N} |i\rangle\langle j| A_{ij}, \qquad A_{ij} = \langle i|\hat{A}|j\rangle,}$$

$$\boxed{\hat{A} = \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dx'\, |x\rangle\langle x'| A(x, x'), \qquad A(x, x') = \langle x|\hat{A}|x'\rangle.}$$

- Why do we do all this? First, it allows us to work with often more "practical" objects – column vectors and matrices (in discrete case) or complex functions and, as you'll see, differential operators (in continuous case) – instead of abstract kets and operators. Second, by an intelligent choice of a basis we can make calculations significantly simpler.

- To get some intuition with representations, let's rewrite some abstract expressions in Dirac notation using representations.

  Let's first take two vectors, $|\psi\rangle$ and $|\phi\rangle$, and consider their inner product, $\langle\psi|\phi\rangle$. Let's pass to the representations of $|\psi\rangle$ and $|\phi\rangle$ in the basis $\{|i\rangle : i=1,2,\dots,N\}$ (discrete case) / $\{|x\rangle : x\in\mathbb{R}\}$ (continuous case), and let's see what happens to $\langle\psi|\phi\rangle$.

I'll show you two ways to get it. First one: You write the representations, $|\psi\rangle = \sum_{i=1}^{N}|i\rangle\psi_i$, $|\phi\rangle=\sum_{j=1}^{N}|j\rangle\phi_j$, you take dual conjugation of $|\psi\rangle$, i.e. $\langle\psi| = \sum_{i=1}^{N}\langle i|\psi_i^*$, and you get:

$$\langle\psi|\phi\rangle = \underbrace{\sum_{i=1}^{N}\sum_{j=1}^{N}\langle i|\,\psi_i^*\phi_j\,|j\rangle}_{\text{(LINEARITY)}} = \sum_{i=1}^{N}\sum_{j=1}^{N}\psi_i^*\phi_j\underbrace{\langle i|j\rangle}_{=\delta_{ij}\ \text{(ORTHONORMALITY)}} = \sum_{i=1}^{N}\psi_i^*\phi_i.$$

Alternatively, you can use the "insertion of identity" technique:

$$\langle\psi|\phi\rangle = \sum_{i=1}^{N}\overbrace{\langle\psi|}^{\text{BRA}}\overbrace{i\rangle\langle i}^{\text{OPERATOR}}\overbrace{|\phi\rangle}^{\text{KET}} = \sum_{i=1}^{N}\psi_i^*\phi_i.$$

$$\underbrace{\langle\psi|i\rangle}_{\text{NUMBER}\ =\psi_i^*}\quad \underbrace{\langle i|\phi\rangle}_{\text{NUMBER}\ =\phi_i}$$

$$\hat{1} = \sum_{i=1}^{N}|i\rangle\langle i|$$

The computation in the continuous case is completely analogous, provided you change summation to integration and Kronecker delta to Dirac delta; for example, using the "insertion of identity", we get:

$$\langle\psi|\phi\rangle = \int_{-\infty}^{+\infty}dx\,\overbrace{\langle\psi|}^{\text{BRA}}\overbrace{x\rangle\langle x}^{\text{OPERATOR}}\overbrace{|\phi\rangle}^{\text{KET}} = \int_{-\infty}^{+\infty}dx\,\psi(x)^*\phi(x).$$

$$\underbrace{\langle\psi|x\rangle}_{\text{NUMBER}\ =\psi(x)^*}\quad \underbrace{\langle x|\phi\rangle}_{\text{NUMBER}\ =\phi(x)}$$

$$\hat{1} = \int_{-\infty}^{+\infty}dx\,|x\rangle\langle x|$$

To sum up:

$$\boxed{\langle\psi|\phi\rangle = \sum_{i=1}^{N}\psi_i^*\phi_i,}$$

$$\boxed{\langle\psi|\phi\rangle = \int_{-\infty}^{+\infty}dx\,\psi(x)^*\phi(x).}$$

We thus see that we've rewritten the abstract expression $\langle\psi|\phi\rangle$ using just the representations of both vectors, i.e. ψ_i and ϕ_i (discrete case) / $\psi(x)$ and $\phi(x)$ (continuous case).

In particular, for $|\phi\rangle=|\psi\rangle$ (using: $z^*z=|z|^2$, for any $z\in\mathbb{C}$):

$$\boxed{\langle\psi|\psi\rangle = \sum_{i=1}^{N}|\psi_i|^2,}$$

$$\boxed{\langle\psi|\psi\rangle = \int_{-\infty}^{+\infty}dx\,|\psi(x)|^2.}$$

- As the second example, let's consider an operator $\hat{A}$ acting on a ket $|\psi\rangle$; this of course produces another ket, let's call it $|\phi\rangle$:

$$\hat{A}|\psi\rangle = |\phi\rangle.$$

Let's rewrite this equation after passing to representations. In the discrete case, we have $\hat{A} = \sum_{i=1}^{N}\sum_{j=1}^{N} |i\rangle\langle j| A_{ij}$, $|\psi\rangle = \sum_{k=1}^{N} |k\rangle \psi_k$, $|\phi\rangle = \sum_{l=1}^{N} |l\rangle \phi_l$, which we plug into the equation:

$$\sum_{i=1}^{N}\sum_{j=1}^{N} |i\rangle\langle j| A_{ij} \sum_{k=1}^{N} |k\rangle \psi_k = \sum_{l=1}^{N} |l\rangle \phi_l$$

$$\sum_{i=1}^{N}\sum_{j=1}^{N}\sum_{k=1}^{N} A_{ij}\psi_k |i\rangle \underbrace{\langle j|k\rangle}_{=\delta_{jk}\ \text{(ORTHONORMALITY)}} = \sum_{l=1}^{N} |l\rangle \phi_l$$

(CHANGE SUMMATION VARIABLE HERE: $l \to i$)

$$\sum_{i=1}^{N}\Big(\sum_{j=1}^{N} A_{ij}\psi_j\Big)|i\rangle = \sum_{i=1}^{N} \phi_i |i\rangle$$

$\downarrow$ ($\{|i\rangle : i = 1,2,\dots,N\}$ IS A BASIS)

$$\sum_{j=1}^{N} A_{ij}\psi_j = \phi_i, \qquad \text{for all } i = 1,2,\dots,N.$$

You recognize this as a matrix equation:

$$\begin{array}{ccccc} N\times N & N\times 1 & & N\times 1 & \\ \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1N} \\ A_{21} & A_{22} & \cdots & A_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ A_{N1} & A_{N2} & \cdots & A_{NN} \end{pmatrix} & \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_N \end{pmatrix} & = & \begin{pmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_N \end{pmatrix}, & \end{array} \qquad \text{or for short} \qquad [A][\psi] = [\phi].$$

You could get the same result also by "insertion of identity" and multiplication by $\langle i|$ from the left:

$$\hat{A}|\psi\rangle = |\phi\rangle \longrightarrow \langle i|\hat{A}|\psi\rangle = \langle i|\phi\rangle$$

$$\uparrow$$

$$1 = \sum_{j=1}^{N} |j\rangle\langle j|$$

$$\downarrow$$

$$\sum_{j=1}^{N} \underbrace{\overbrace{\langle i|}^{\text{BRA}}\overbrace{\hat{A}}^{\text{OPER.}}|j\rangle}_{\text{NUMBER} = A_{ij}} \underbrace{\overbrace{\langle j|\psi\rangle}^{\text{OPERATOR KET}}}_{\text{NUMBER} = \psi_j} = \underbrace{\langle i|\phi\rangle}_{\text{NUMBER} = \phi_i}$$

$$\downarrow$$

$$\sum_{j=1}^{N} A_{ij}\psi_j = \phi_i.$$

Proceeding analogously in the continuous case (check if you're in doubt!), we finally find that the abstract equation:

$$\boxed{\hat{A}|\psi\rangle = |\phi\rangle}$$

can be rewritten as a matrix equation (discrete case):

$$\sum_{j=1}^{N} A_{ij}\psi_j = \phi_i, \quad \text{for all } i = 1,2,\dots,N,$$

which is:

$$\begin{pmatrix} A_{11} & A_{12} & \dots & A_{1N} \\ \vdots & \vdots & \ddots & \vdots \\ A_{N1} & A_{N2} & \dots & A_{NN} \end{pmatrix}\begin{pmatrix}\psi_1 \\ \vdots \\ \psi_N\end{pmatrix} = \begin{pmatrix}\phi_1 \\ \vdots \\ \phi_N\end{pmatrix}, \quad \text{i.e. } [A][\psi] = [\phi],$$

or as an integral equation (continuous case):

$$\int_{-\infty}^{+\infty} dx' A(x,x')\,\psi(x') = \phi(x), \quad \text{for all } x \in \mathbb{R}.$$

CHANGE OF A REPRESENTATION OF A KET

- Let's choose a ket $|\psi\rangle$. We emphasized before that it's a meaningful object even before any basis is chosen. If we now pick some basis in our vector space (an orthonormal one), we can find the representation of $|\psi\rangle$ in this basis $\{|i\rangle : i=1,2,\dots,N\}$ (discrete case) / $\{|x\rangle : x\in\mathbb{R}\}$ (continuous case):

$$|\psi\rangle = \sum_{i=1}^{N} |i\rangle \underbrace{\langle i|\psi\rangle}_{\psi_i} \qquad\qquad |\psi\rangle = \int_{-\infty}^{+\infty} dx\, |x\rangle \underbrace{\langle x|\psi\rangle}_{\psi(x)}.$$

Now let's choose another orthonormal basis $\{|\tilde{i}\rangle : i=1,2,\dots,N\}$ (discrete case) / $\{|\tilde{x}\rangle : x\in\mathbb{R}\}$ (continuous case); the representation of the ket $|\psi\rangle$ in this new basis is:

$$|\psi\rangle = \sum_{i=1}^{N} |\tilde{i}\rangle \underbrace{\langle \tilde{i}|\psi\rangle}_{\tilde{\psi}_i} \qquad\qquad |\psi\rangle = \int_{-\infty}^{+\infty} dx\, |\tilde{x}\rangle \underbrace{\langle \tilde{x}|\psi\rangle}_{\tilde{\psi}(x)}.$$

The question is: How can we find the new representation $\tilde{\psi}_i$ / $\tilde{\psi}(x)$ provided we know the old representation?

The solution is easy when we use our basic technique in Dirac notation, i.e. the "insertion of identity":

$$\tilde{\psi}_i = \widetilde{\langle i|}\psi\rangle = \sum_{j=1}^{N} \underbrace{\overbrace{\widetilde{\langle i|}}^{\text{BRA}}\overbrace{j\rangle\langle j}^{\text{OPERATOR}}}_{\text{NUMBER}}\underbrace{\overbrace{|\psi\rangle}^{\text{KET}}}_{\text{NUMBER} = \psi_j} = \sum_{j=1}^{N} U_{ij}\,\psi_j\,,$$

$$\hat{1} = \sum_{j=1}^{N} |j\rangle\langle j|$$

where by U_{ij} we denoted inner product between the "new basis" vector $\widetilde{|i\rangle}$ and the "old basis" vector $|j\rangle$, $U_{ij} \equiv \widetilde{\langle i|}j\rangle$; all such inner products must be known in order to perform change of representation. Exactly the same way works in the continuous case:

$$\tilde{\psi}(x) = \widetilde{\langle x|}\psi\rangle = \int_{-\infty}^{+\infty} dx' \underbrace{\overbrace{\widetilde{\langle x|}}^{\text{BRA}}\overbrace{x'\rangle\langle x'}^{\text{OPERATOR}}}_{\text{NUMBER}}\underbrace{\overbrace{|\psi\rangle}^{\text{KET}}}_{\text{NUMBER} = \psi(x')} = \int_{-\infty}^{+\infty} dx'\, U(x,x')\,\psi(x'),$$

$$\hat{1} = \int_{-\infty}^{+\infty} dx' |x'\rangle\langle x'|$$

with $U(x,x') \equiv \widetilde{\langle x|}x'\rangle$.

To sum up:

$$\boxed{\begin{array}{l} \tilde{\psi}_i = \sum_{j=1}^{N} U_{ij}\,\psi_j\,, \quad \text{for all } i = 1,2,\dots,N, \quad U_{ij} \equiv \widetilde{\langle i|}j\rangle, \\ \text{which is:} \\ \begin{pmatrix} \tilde{\psi}_1 \\ \tilde{\psi}_2 \\ \vdots \\ \tilde{\psi}_N \end{pmatrix} = \begin{pmatrix} U_{11} & U_{12} & \cdots & U_{1N} \\ U_{21} & U_{22} & \cdots & U_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ U_{N1} & U_{N2} & \cdots & U_{NN} \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_N \end{pmatrix}, \quad \text{i.e.} \quad [\tilde{\psi}] = [U][\psi], \end{array}}$$

$$\boxed{\tilde{\psi}(x) = \int_{-\infty}^{+\infty} dx'\, U(x,x')\,\psi(x'), \quad \text{for all } x \in \mathbb{R}, \quad U(x,x') \equiv \widetilde{\langle x|}x'\rangle.}$$

And we were able to obtain these results very quickly because of the use of the "insertion of identity" technique – you see again how useful it is.

- Let's show now, as an exercise that the transition matrix $[U]$ / $U(x,x')$ is unitary. For the $N\times N$ matrix $[U]$, "unitary" means:

$$\boxed{[U]^{\dagger}[U] = [1], \quad \text{i.e.} \quad \sum_{k=1}^{N} U_{ki}^{*}\,U_{kj} = \delta_{ij},}$$

while, by analogy, in the case of $U(x,x')$ it means:

$$\boxed{\int_{-\infty}^{+\infty} dx''\, U(x'',x)^* U(x'',x') = \delta(x-x').}$$

Proof in the discrete case:

$$\sum_{k=1}^{N} U_{ki}^* U_{kj} = \sum_{k=1}^{N} \langle \tilde{k}|i\rangle^* \langle \tilde{k}|j\rangle = \sum_{k=1}^{N} \overbrace{\underbrace{\langle i|}_{\text{BRA}}\tilde{k}\rangle}^{\text{NUMBER}} \overbrace{\langle\tilde{k}|\underbrace{j\rangle}_{\text{KET}}}^{\text{NUMBER}} = \langle i|j\rangle = \delta_{ij}.$$

(WE USE $\langle\alpha|\beta\rangle^* = \langle\beta|\alpha\rangle$)

OPERATOR (THE OPERATOR $\sum_{k=1}^{N} |\tilde{k}\rangle\langle\tilde{k}|$ IS JUST $\hat{1}$, SO WE CAN FORGET ABOUT IT)

(ORTHONORMALITY)

In the continuous case it goes identically the same, but let me write it down so that you get more acquainted with continuous bases:

$$\int_{-\infty}^{+\infty} dx''\, U(x'',x)^* U(x'',x') = \int_{-\infty}^{+\infty} dx'' \langle\widetilde{x''}|x\rangle^* \langle\widetilde{x''}|x'\rangle =$$

$$= \int_{-\infty}^{+\infty} dx'' \overbrace{\underbrace{\langle x|}_{\text{BRA}}\widetilde{x''}\rangle}^{\text{NUMBER}} \overbrace{\langle\widetilde{x''}|\underbrace{x'\rangle}_{\text{KET}}}^{\text{NUMBER}} = \langle x|x'\rangle = \delta(x-x').$$

OPERATOR ($\int_{-\infty}^{+\infty} dx'' |\widetilde{x''}\rangle\langle\widetilde{x''}| = \hat{1}$)

(ORTHONORMALITY)

Notice that this time we "removed" identity $\hat{1}$ (composed out of the vectors of the "new basis"); again you see that you <u>must</u> know by heart the completeness relation.

- Example: Problem 2.7. Here we have 2-dimensional vector space ($N=2$), and in it we choose two orthonormal bases: the "old basis" is denoted by $\{|+\rangle, |-\rangle\}$ (in our notation: $|1\rangle = |+\rangle$, $|2\rangle = |-\rangle$), and the "new basis" is $\{|S_x,+\rangle, |S_x,-\rangle\}$ (in our notation: $|\tilde{1}\rangle = |S_x,+\rangle$, $|\tilde{2}\rangle = |S_x,-\rangle$), and we're told that $|S_x,\pm\rangle = \frac{1}{\sqrt{2}}(|+\rangle \pm |-\rangle)$. We're given a ket $|S_y,+\rangle$ (in our notation: $|\psi\rangle = |S_y,+\rangle$), and we know its representation in the "old basis", $|S_y,+\rangle = \frac{1}{\sqrt{2}}(|+\rangle + i|-\rangle) \leftrightarrow \begin{pmatrix}1/\sqrt{2}\\ i/\sqrt{2}\end{pmatrix}$ (in our notation: $\psi_1 = \frac{1}{\sqrt{2}}$, $\psi_2 = \frac{i}{\sqrt{2}}$, i.e. the representation is $\begin{pmatrix}1/\sqrt{2}\\ i/\sqrt{2}\end{pmatrix}$). We want to find its representation in the "new basis" (in our notation: $\begin{pmatrix}\tilde{\psi}_1\\ \tilde{\psi}_2\end{pmatrix}$).

So we must find the transition matrix $[U] = \begin{pmatrix}U_{11} & U_{12}\\ U_{21} & U_{22}\end{pmatrix}$. We have:

$$U_{11} = \langle\tilde{1}|1\rangle = \langle S_x,+|+\rangle = \tfrac{1}{\sqrt{2}}(\langle+|+\langle-|)\,|+\rangle = \tfrac{1}{\sqrt{2}}\big(\underbrace{\langle+|+\rangle}_{=1} + \underbrace{\langle-|+\rangle}_{=0}\big) = \tfrac{1}{\sqrt{2}},$$

$$U_{12} = \langle\tilde{1}|2\rangle = \langle S_x,+|-\rangle = \tfrac{1}{\sqrt{2}}(\langle+|+\langle-|)\,|-\rangle = \tfrac{1}{\sqrt{2}}\big(\underbrace{\langle+|-\rangle}_{=0} + \underbrace{\langle-|-\rangle}_{=1}\big) = \tfrac{1}{\sqrt{2}},$$

$$U_{21} = \langle\tilde{2}|1\rangle = \langle S_x,-|+\rangle = \tfrac{1}{\sqrt{2}}(\langle+|-\langle-|)\,|+\rangle = \tfrac{1}{\sqrt{2}}\big(\underbrace{\langle+|+\rangle}_{=1} - \underbrace{\langle-|+\rangle}_{=0}\big) = \tfrac{1}{\sqrt{2}},$$

$$U_{22} = \langle\tilde{2}|2\rangle = \langle S_x,-|-\rangle = \tfrac{1}{\sqrt{2}}(\langle+|-\langle-|)\,|-\rangle = \tfrac{1}{\sqrt{2}}\big(\underbrace{\langle+|-\rangle}_{=0} - \underbrace{\langle-|-\rangle}_{=1}\big) = -\tfrac{1}{\sqrt{2}},$$

(ORTHONORMALITY)

i.e.:

$$[U] = \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & -1/\sqrt{2} \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

Before we proceed, let's check that $[U]$ is unitary:

$$[U]^\dagger [U] = \overset{2\times2}{\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}}\ \overset{2\times2}{\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}} = \overset{2\times2}{\frac{1}{2}\begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = [1].$$

Hence the new representation:

$$\begin{pmatrix} \langle S_x,+|S_y,+\rangle \\ \langle S_x,-|S_y,+\rangle \end{pmatrix} = \underbrace{\begin{pmatrix} \langle\tilde{1}|\psi\rangle \\ \langle\tilde{2}|\psi\rangle \end{pmatrix} = [\tilde{\psi}]}_{\text{(OUR NOTATION)}} \overset{\text{(THE FORMULA FOR CHANGE OF REPRESENTATION OF A KET)}}{=} [U][\psi] = \overset{2\times2}{\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}}\ \overset{2\times1}{\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}} = \overset{2\times1}{\frac{1}{2}\begin{pmatrix} 1+i \\ 1-i \end{pmatrix}}.$$

This is the new representation: $\tilde{\varphi}_1 = \frac{1+i}{2}$, $\tilde{\varphi}_2 = \frac{1-i}{2}$. Using $|\psi\rangle = \sum_{i=1}^{N} |\tilde{i}\rangle \tilde{\varphi}_i$, we can write it as:

$$|S_y,+\rangle = \frac{1+i}{2}|S_x,+\rangle + \frac{1-i}{2}|S_x,-\rangle.$$

- Example: A ket in the position and momentum bases. You'll later learn about the so-called <u>position basis</u> and <u>momentum basis</u> in QM. Now let's not define them, but let's just state that they are two continuous bases:

$$\boxed{\begin{matrix} \{|x\rangle : x \in \mathbb{R}\}, \\ \{|p\rangle : p \in \mathbb{R}\}, \end{matrix}}$$

and that the transition "matrix" between them is given by:

$$\boxed{U(p,x) = \langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}}\, e^{-\frac{i}{\hbar}px}.}$$

(In the opposite way it's of course: $\boxed{\langle x|p\rangle = \langle p|x\rangle^* = \frac{1}{\sqrt{2\pi\hbar}}\, e^{+\frac{i}{\hbar}px}}$.)

Let's pick an arbitrary ket $|\psi\rangle$. Its representations in the two above bases we know very well how to write:

$$\boxed{\begin{aligned} |\psi\rangle &= \int_{-\infty}^{+\infty} dx\, |x\rangle\, \psi(x), \qquad & \psi(x) &= \langle x|\psi\rangle, \\ |\psi\rangle &= \int_{-\infty}^{+\infty} dp\, |p\rangle\, \psi(p), \qquad & \psi(p) &= \langle p|\psi\rangle. \end{aligned}}$$

The function $\psi(x)$ is in QM called <u>the position wavefunction</u>, while the function $\psi(p)$ <u>the momentum wavefunction</u>.

What's a relation between the position and momentum wavefunctions? By the general formula:

$$\boxed{\psi(p) = \int_{-\infty}^{+\infty} dx\, U(p,x)\, \psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} dx\, e^{-\frac{i}{\hbar}px}\, \psi(x).}$$

In the opposite way:

$$\boxed{\psi(x) = \int_{-\infty}^{+\infty} dp\, U'(x,p)\, \psi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} dp\, e^{+\frac{i}{\hbar}px}\, \psi(p).}$$

$\leftarrow \left(U'(x,p) = \langle x|p\rangle = \langle p|x\rangle^* = \frac{1}{\sqrt{2\pi\hbar}} e^{+\frac{i}{\hbar}px}\right)$

This kind of a relation is called in mathematics <u>"Fourier transformation"</u>.

You may ask if the transition "matrix" $U(p,x) = \frac{1}{\sqrt{2\pi\hbar}} e^{-\frac{i}{\hbar}px}$ is unitary, i.e. if it satisfies:

$$\int_{-\infty}^{+\infty} dp\, U(p,x)^* U(p,x') = \boxed{\frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} dp\, e^{\frac{i}{\hbar}p(x-x')} = \delta(x-x').}$$

Though we won't do it, this formula can be proven. And it's important you remember it!

It's good to practice this passage between the position and momentum bases. Warm-Up Problem 4.2 provides such a practical example. Here you are given a normalized position wavefunction $\psi(x) = \frac{1}{\sqrt{s}} e^{-\frac{|x|}{s}}$, for some $s>0$, and you're asked to find the corresponding momentum wavefunction. We have:

$$\psi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} dx\, e^{-\frac{i}{\hbar}px}\, \psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} dx\, e^{-\frac{i}{\hbar}px} \frac{1}{\sqrt{s}} e^{-\frac{|x|}{s}} = \left\{ \begin{array}{l} \text{FOR } x \in \mathbb{R}: \\ |x| = \begin{cases} x, & \text{IF } x \geq 0 \\ -x, & \text{IF } x \leq 0 \end{cases} \end{array} \right\}$$

$$= \frac{1}{\sqrt{2\pi\hbar s}} \left(\int_0^{+\infty} dx\, e^{-\frac{i}{\hbar}px - \frac{1}{s}x} + \int_{-\infty}^{0} dx\, e^{-\frac{i}{\hbar}px + \frac{1}{s}x} \right) = \left\{ \begin{array}{c} \text{CHANGE OF VARIABLES} \\ x \to -x \text{ IN THE SECOND} \\ \text{INTEGRAL} \end{array} \right\} =$$

$$= \frac{1}{\sqrt{2\pi\hbar s}}\left(\int_0^{+\infty} dx\, e^{-\left(\frac{i}{\hbar}p+\frac{1}{s}\right)x} + \int_0^{+\infty} dx\, e^{-\left(-\frac{i}{\hbar}p+\frac{1}{s}\right)x}\right) =$$

$$= \left\{\begin{array}{l}\text{WE USE HERE } \int_0^{+\infty} dx\, e^{-\alpha x} = \frac{1}{\alpha}, \\ \text{WHICH IS TRUE FOR } \alpha \in \mathbb{R}_+, \text{ BUT} \\ \text{WHICH HOWEVER GIVES THE RIGHT} \\ \text{RESULT EVEN IF } \alpha \in \mathbb{C} \text{ AND } \mathrm{Re}(\alpha) > 0\end{array}\right\} =$$

$$= \frac{1}{\sqrt{2\pi\hbar s}}\left(\frac{\hbar s}{\hbar + ips} + \frac{\hbar s}{\hbar - ips}\right) = \sqrt{\frac{2s}{\pi\hbar}}\,\frac{1}{1+\frac{p^2 s^2}{\hbar^2}}.$$

Hence we see that the position wavefunction $\psi(x) = \frac{1}{\sqrt{s}} e^{-\frac{|x|}{s}}$ corresponds to the momentum wavefunction $\psi(p) = \sqrt{\frac{2s}{\pi\hbar}}\frac{1}{1+\frac{p^2 s^2}{\hbar^2}}$.

CHANGE OF A REPRESENTATION OF AN OPERATOR

- Analogously we find how to change representation of an operator $\hat{A}$. In the "old basis":

$$\hat{A} = \sum_{i=1}^{N}\sum_{j=1}^{N} |i\rangle \underbrace{\langle i|\hat{A}|j\rangle}_{A_{ij}} \langle j| \qquad \hat{A} = \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dx'\, |x\rangle \underbrace{\langle x|\hat{A}|x'\rangle}_{A(x,x')} \langle x'|,$$

while in the "new basis":

$$\hat{A} = \sum_{i=1}^{N}\sum_{j=1}^{N} |\tilde{i}\rangle \underbrace{\langle\tilde{i}|\hat{A}|\tilde{j}\rangle}_{\tilde{A}_{ij}} \langle\tilde{j}| \qquad \hat{A} = \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dx'\, |\tilde{x}\rangle \underbrace{\langle\tilde{x}|\hat{A}|\tilde{x}'\rangle}_{\tilde{A}(x,x')} \langle\tilde{x}'|.$$

By inserting the identity twice we get:

$$\tilde{A}_{ij} = \langle\tilde{i}|\hat{A}|\tilde{j}\rangle = \sum_{k=1}^{N}\sum_{l=1}^{N} \underbrace{\overbrace{\langle\tilde{i}|}^{\text{BRA}}\overbrace{k\rangle\langle k|}^{\text{OPERATOR}}}_{\text{NUMBER}}\underbrace{\overbrace{\hat{A}}^{\text{OPERATOR}}}_{\text{NUMBER}}\underbrace{\overbrace{|l\rangle\langle l|}^{\text{OPERATOR}}\overbrace{\tilde{j}\rangle}^{\text{KET}}}_{\text{NUMBER}} = \sum_{k=1}^{N}\sum_{l=1}^{N} U_{ik} A_{kl} U^*_{jl}$$

$$\hat{1} = \sum_{l=1}^{N} |l\rangle\langle l| \qquad \hat{1} = \sum_{k=1}^{N} |k\rangle\langle k|$$

where $[U]$ is the above-defined transition matrix, $U_{ij} = \langle\tilde{i}|j\rangle$. In the continuous case the computation is identical, and finally we get:

$$\tilde{A}_{ij} = \sum_{k=1}^{N}\sum_{l=1}^{N} \underbrace{U_{ik}}_{=\tilde{\langle i}|k\rangle} A_{kl} \underbrace{U^*_{jl}}_{=\langle l|\tilde{j}\rangle}, \quad \text{for all } i,j = 1,2,\dots,N,$$

which is:

$$[\tilde{A}] = [U][A][U]^\dagger,$$

$$\tilde{A}(x,x') = \int_{-\infty}^{+\infty} dx'' \int_{-\infty}^{+\infty} dx''' \underbrace{U(x,x'')}_{=\tilde{\langle x}|x''\rangle} A(x'',x''') \underbrace{U(x',x''')^*}_{=\langle x'''|\tilde{x'}\rangle}.$$

These are the formulas for <u>change of representation of an operator $\hat{A}$</u>. You don't necessarily need to remember them - if you remember how to quickly obtain them by "insertion of identity"! Again, you see that "insertion of identity" is a crucial technique in the Dirac notation framework.

• Example: Consider our familiar case of the 2-dimensional ($N=2$) vector space. Let the "old basis" be $\{|+\rangle, |-\rangle\}$, and let the "new basis" be $\{|S_x,+\rangle, |S_x,-\rangle\}$ (like in Problem 2.7). Consider now the operator $\hat{S}_y$. We know that its representation in the "old basis" is $[S_y] = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0\end{pmatrix}$ (see formula (3.12) in the textbook). Find its representation in the "new basis".

We have already found the transition matrix (see p. 15):

$$[U] = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1\end{pmatrix}.$$

Hence:

$$[\tilde{S}_y] = [U][S_y][U]^\dagger = \underbrace{\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1\end{pmatrix}}^{2\times 2} \underbrace{\frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0\end{pmatrix}}^{2\times 2} \underbrace{\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1\end{pmatrix}}^{2\times 2} = \underbrace{\frac{\hbar}{4}\begin{pmatrix} 0 & 2i \\ -2i & 0\end{pmatrix}}^{2\times 2} =$$

$$= \frac{\hbar}{2}\begin{pmatrix} 0 & i \\ -i & 0\end{pmatrix}.$$

Similarly (check if you want!), starting from $[S_x] = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0\end{pmatrix}$ and $[S_z] = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1\end{pmatrix}$, we find: $[\tilde{S}_x] = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1\end{pmatrix}$ and $[\tilde{S}_z] = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0\end{pmatrix}$. You can practice this further by finding the representations of the operators $\hat{S}_x, \hat{S}_y, \hat{S}_z$ in the basis $\{|S_y,+\rangle, |S_y,-\rangle\}$.

• Example: Part of Problem 4.1, <u>the position operator in the momentum basis.</u> Consider now as the "old basis" the position basis $\{|x\rangle : x \in \mathbb{R}\}$, and as the "new basis" the momentum basis $\{|p\rangle : p \in \mathbb{R}\}$. Let's consider also the so-called <u>position operator</u> $\hat{x}$, which here let's define by stating that its representation in the position basis is:

$$\boxed{\langle x|\hat{x}|x'\rangle = x'\,\delta(x-x').}$$

(In other words, $\hat{x} = \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dx'\, |x\rangle\langle x|\hat{x}|x'\rangle\langle x'| = \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dx'\,|x\rangle\langle x'|\, x'\,\delta(x-x') = \int_{-\infty}^{+\infty} dx\, |x\rangle\langle x|\, x.$) What's its representation in the momentum basis?

Assume also that you forgot the formula for change of representation of an operator, but you remember that it's obtained by inserting the identity twice. Then it's not hard to guess how to proceed:

$$\langle p|\hat{x}|p'\rangle = \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dx'\, \underbrace{\overbrace{\langle p|}^{\text{BRA}}\overbrace{x\rangle}^{\text{OPERATOR}}}_{\substack{\text{NUMBER} \\ \parallel \\ \frac{1}{\sqrt{2\pi\hbar}} e^{-\frac{i}{\hbar}px}}} \underbrace{\overbrace{\langle x|}^{\text{OPERATOR}}\overbrace{\hat{x}}^{\text{OPER.}}\overbrace{|x'\rangle}^{\text{OPERATOR}}}_{\substack{\text{NUMBER} \\ \parallel \\ x'\delta(x-x')}} \underbrace{\langle x'|\overbrace{p'\rangle}^{\text{KET}}}_{\substack{\text{NUMBER} \\ \parallel \\ \frac{1}{\sqrt{2\pi\hbar}} e^{+\frac{i}{\hbar}p'x'}}} =$$

$$\hat{1} = \int_{-\infty}^{+\infty} dx'\, |x'\rangle\langle x'|$$

$$\hat{1} = \int_{-\infty}^{+\infty} dx\, |x\rangle\langle x|$$

$$= \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dx'\, \frac{1}{\sqrt{2\pi\hbar}} e^{-\frac{i}{\hbar}px} \cdot x'\,\delta(x-x') \cdot \frac{1}{\sqrt{2\pi\hbar}} e^{+\frac{i}{\hbar}p'x'} =$$

$$= \left\{ \begin{array}{l} \text{DIRAC DELTA } \delta(x-x') \text{ KILLS} \\ \text{ONE OF THE INTEGRALS,} \\ \text{SAY OVER } x', \text{ CAUSING US} \\ \text{TO SUBSTITUTE } x' = x \end{array} \right\} =$$

$$= \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} dx\; x\, e^{\frac{i}{\hbar}x(p'-p)} = \ldots$$

Now to compute this integral you need <u>a trick which is widely used in physics</u>; namely, we notice that:

$$\boxed{\frac{d}{dp'}\left(e^{\frac{i}{\hbar}x(p'-p)}\right) = \frac{i}{\hbar} x\, e^{\frac{i}{\hbar}x(p'-p)}}$$

(derivative over p' "brought down" x from the exponent). Hence:

$$\ldots = \frac{1}{2\pi\hbar}\, \frac{\hbar}{i} \int_{-\infty}^{+\infty} dx\, \frac{d}{dp'}\left(e^{\frac{i}{\hbar}x(p'-p)}\right) = \left\{ \begin{array}{l} \text{WE MOVE DERIVATIVE} \\ \text{BEFORE THE INTEGRAL,} \\ \text{AND WRITE ALSO } \frac{1}{i} = -i, \\ \text{WHICH EASILY STEMS FROM } i^2 = -1 \end{array} \right\} =$$

$$= -i\hbar \frac{d}{dp'}\underbrace{\left(\frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} dx\, e^{\frac{i}{\hbar}x(p'-p)}\right)}_{=\delta(p'-p)} =$$

(REMEMBER THE FORMULA FROM P. 16?)

$$= -i\hbar \frac{d}{dp'}\left(\delta(p'-p)\right).$$

This is the result: the position operator $\hat{x}$, which in the position basis $\{|x\rangle : x \in \mathbb{R}\}$ has the representation $\langle x|\hat{x}|x'\rangle = x'\delta(x-x')$, in the momentum basis $\{|p\rangle : p \in \mathbb{R}\}$ has the representation:

$$\boxed{\langle p|\hat{x}|p'\rangle = -i\hbar \frac{d}{dp'}\left(\delta(p'-p)\right),}$$

i.e. it is a constant $(-i\hbar)$ times derivative of Dirac delta $\delta(p'-p)$ over p'; yes, it's a very strange function of two variables, but below I'll show you how to practically deal with it.

This is how the above two representations of $\hat{x}$ are used practically: You've seen on p. 11–12 that you can rewrite an abstract equation $\hat{A}|\psi\rangle = |\phi\rangle$ in a given representation: $[A]\begin{pmatrix}\psi_1\\ \vdots \\ \psi_N\end{pmatrix} = \begin{pmatrix}\phi_1\\ \vdots \\ \phi_N\end{pmatrix}$ (discrete case) / $\int_{-\infty}^{+\infty} dx'\, A(x,x')\,\psi(x') = \phi(x)$ (continuous case). Let's do this for the position operator $\hat{x}$, first using the position basis, second using the momentum basis. And let's again assume you forgot the formula, but you remember that it's obtained by "insertion of identity."

So the first task is to write $\hat{x}|\psi\rangle$, for an arbitrary ket $|\psi\rangle$, in the position representation:

$$\underset{\uparrow \atop \hat{1}=\int_{-\infty}^{+\infty}dx'|x'\rangle\langle x'|}{\langle x|\hat{x}|\psi\rangle} = \int_{-\infty}^{+\infty} dx' \underbrace{\overbrace{\langle x|}^{\text{BRA}}\overbrace{\hat{x}}^{\text{OPERATOR}}|x'\rangle}_{\substack{\text{NUMBER}\\ =x'\delta(x-x')}} \underbrace{\overbrace{\langle x'|}^{\text{OPERATOR}}\overbrace{\psi\rangle}^{\text{KET}}}_{\substack{\text{NUMBER}\\ =\psi(x')}} = \int_{-\infty}^{+\infty} dx'\; x'\delta(x-x')\cdot\psi(x') =$$

$$= \left\{\begin{matrix}\text{DIRAC DELTA } \delta(x-x') \\ \text{KILLS THE INTEGRAL,} \\ \text{AND SETS } x'=x\end{matrix}\right\} = x\psi(x),$$

i.e. the action of $\hat{x}$ on an arbitrary ket $|\psi\rangle$, $|\phi\rangle = \hat{x}|\psi\rangle$, is written in the position representation as:

$$\boxed{\phi(x) = \langle x|\hat{x}|\psi\rangle = x\,\psi(x),}$$

i.e. the action of the position operator $\hat{x}$ on an arbitrary ket $|\psi\rangle$ is in the position representation just the multiplication of $\psi(x)$ by x.

OK, so now let's repeat this for the momentum representation, i.e. let's find $\phi(p) = \langle p|\phi\rangle = \langle p|\hat{x}|\psi\rangle$:

$$\underset{\uparrow\ \hat{1} = \int_{-\infty}^{+\infty} dp'|p'\rangle\langle p'|}{\langle p|\hat{x}|\psi\rangle} = \int_{-\infty}^{+\infty} dp' \underbrace{\overbrace{\langle p|}^{\text{BRA}}\overbrace{\hat{x}}^{\text{OPER}}\overbrace{|p'\rangle}^{\text{OPERATOR}}}_{\substack{\text{NUMBER} \\ = -i\hbar\frac{d}{dp'}(\delta(p'-p))}} \underbrace{\overbrace{\langle p'|\psi\rangle}^{\text{KET}}}_{\substack{\text{NUMBER} \\ = \psi(p')}} = \int_{-\infty}^{+\infty} dp' (-i\hbar)\frac{d}{dp'}\left(\delta(p'-p)\right)\cdot\psi(p') = \ldots$$

We have here that weird function $\frac{d}{dp'}(\delta(p'-p))$ (derivative of Dirac delta) and how should we handle it? By integration by parts – integration by parts is the usual way of handling derivative of Dirac delta. Recall that integration by parts reads:

$$\boxed{\int_{-\infty}^{+\infty} dy\, \frac{df(y)}{dy}\, g(y) = f(y)g(y)\Big|_{y=-\infty}^{y=+\infty} - \int_{-\infty}^{+\infty} dy\, f(y)\frac{dg(y)}{dy},}$$

but in QM we consider only wavefunctions that vanish at $\pm\infty$, hence in most cases in QM you'll have: $\boxed{f(y)g(y)\Big|_{y=-\infty}^{y=+\infty} = 0}$. This is the case here:

$$\ldots = \underset{\substack{\uparrow \\ \text{(CHANGE OF SIGN DUE} \\ \text{TO INTEGRATION BY PARTS)}}}{+}i\hbar \int_{-\infty}^{+\infty} dp'\, \delta(p'-p)\,\frac{d\psi(p')}{dp'} = \left\{\begin{matrix}\text{DIRAC DELTA } \delta(p'-p) \\ \text{KILLS THE INTEGRAL,} \\ \text{AND SETS } p'=p\end{matrix}\right\} =$$

$$= i\hbar\,\frac{d\psi(p)}{dp},$$

i.e. the action of $\hat{x}$ on an arbitrary ket $|\psi\rangle$, $|\phi\rangle = \hat{x}|\psi\rangle$, is written in the momentum representation as:

$$\boxed{\psi(p) = \langle p|\hat{x}|\psi\rangle = +i\hbar \frac{d}{dp}\psi(p),}$$

i.e. the action of the position operator $\hat{x}$ on an arbitrary ket $|\psi\rangle$ is in the momentum representation the differentiation of $\psi(p)$ times the constant $i\hbar$.

The above two results, $\langle x|\hat{x}|\psi\rangle = x\psi(x)$ and $\langle p|\hat{x}|\psi\rangle = i\hbar\frac{d}{dp}\psi(p)$, are the reason for the following widely-spread terminology: Even though formally speaking, the representation of $\hat{x}$ in the position basis is a function of two variables x, x' and the representation of $\hat{x}$ in the momentum basis is a function of two variables p, p':

$$\boxed{\begin{aligned} &\langle x|\hat{x}|x'\rangle = x'\delta(x-x'), \\ &\langle p|\hat{x}|p'\rangle = -i\hbar\frac{d(\delta(p'-p))}{dp'}, \end{aligned}}$$

(compare p. 8: the representation of an operator $\hat{A}$ in a continuous basis $\{|x\rangle : x \in \mathbb{R}\}$ — don't confuse this with the position basis!, it's an arbitrary continuous basis and I just used the same letter "x" — is a function of two variables x, x', namely $A(x,x') = \langle x|\hat{A}|x'\rangle$), however practically speaking, what is normally called "the representation of $\hat{x}$ in the position basis" is the operator of multiplication by number x, and what is normally called "the representation of $\hat{x}$ in the momentum basis" is the constant $i\hbar$ times the operator of differentiation over p, i.e. $i\hbar\frac{d}{dp}$, which we denote by:

$$\boxed{\begin{aligned} &\hat{x} \xrightarrow{\{|x\rangle\}} x, \\ &\hat{x} \xrightarrow{\{|p\rangle\}} i\hbar\frac{d}{dp}. \end{aligned}}$$

(Notice that these "operators" are not operators in our abstract vector space, but rather they're operators in the space of position/momentum wave-functions, i.e. they act on $\psi(x)$ and $\psi(p)$ respectively, not on $|\psi\rangle$.)

• Example: In precisely the same way, you can try to repeat the above calculation in the case of <u>the momentum operator $\hat{p}$</u>, which here we define by giving its representation in the momentum basis:

$$\boxed{\langle p|\hat{p}|p'\rangle = p'\delta(p-p').}$$

Find that its representation in the position basis is:

$$\boxed{\langle x|\hat{p}|x'\rangle = +i\hbar\frac{d(\delta(x'-x))}{dx'}}$$

(notice sign change with respect to $\langle p|\hat{x}|p'\rangle$). These are both functions of two variables, as is formally right. But show that the action of $\hat{p}$ on an arbitrary ket $|\psi\rangle$, $\hat{p}|\psi\rangle = |\phi\rangle$, can be written in our two bases as:

$$\boxed{\begin{aligned}\langle x|\hat{p}|\psi\rangle &= -i\hbar\frac{d}{dx}\psi(x),\\ \langle p|\hat{p}|\psi\rangle &= p\psi(p)\end{aligned}}$$

(notice sign change in $\langle x|\hat{p}|\psi\rangle$ with respect to $\langle p|\hat{x}|\psi\rangle$), which amounts for the common terminology:

$$\boxed{\begin{aligned}\hat{p} &\xrightarrow{\{|x\rangle\}} -i\hbar\frac{d}{dx},\\ \hat{p} &\xrightarrow{\{|p\rangle\}} p.\end{aligned}}$$

• Example: Let's show now a little more of how to practically use the above representations of $\hat{x}$ and $\hat{p}$ in the position and momentum bases, <u>in the more practical form of differential operators</u> (not functions of two variables). To this end, let's compute the commutator $[\hat{x},\hat{p}]$, which we know to be $[\hat{x},\hat{p}] = i\hbar\hat{1}$, in both representations. (You find this task also in Problem 4.1.)

In the position representation, $\hat{x} \xrightarrow{\{|x\rangle\}} x$ and $\hat{p} \xrightarrow{\{|x\rangle\}} -i\hbar\frac{d}{dx}$, hence for an arbitrary ket $|\psi\rangle$:

$$[\hat{x}, \hat{p}]|\psi\rangle \xrightarrow{\{|x\rangle\}} x\left(-i\hbar\frac{d}{dx}\right)\psi(x) - \left(-i\hbar\frac{d}{dx}\right)x\psi(x) =$$

$$= -i\hbar\, x\frac{d\psi(x)}{dx} + i\hbar\frac{d(x\psi(x))}{dx} =$$

$$= \cancel{-i\hbar\, x\frac{d\psi(x)}{dx}} + i\hbar\psi(x) + \cancel{i\hbar\, x\frac{d\psi(x)}{dx}} =$$

$$= i\hbar\psi(x),$$

and of course $i\hbar\hat{1}|\psi\rangle \xrightarrow{\{|x\rangle\}} i\hbar\psi(x)$, hence we proved $[\hat{x}, \hat{p}] = i\hbar\hat{1}$ in the position basis.

Similarly, in the momentum representation, $\hat{x} \xrightarrow{\{|p\rangle\}} i\hbar\frac{d}{dp}$ and $\hat{p} \xrightarrow{\{|p\rangle\}} p$, hence for arbitrary $|\psi\rangle$:

$$[\hat{x}, \hat{p}]|\psi\rangle \xrightarrow{\{|p\rangle\}} \left(i\hbar\frac{d}{dp}\right)p\psi(p) - p\left(i\hbar\frac{d}{dp}\right)\psi(p) =$$

$$= i\hbar\frac{d(p\psi(p))}{dp} - i\hbar p\frac{d\psi(p)}{dp} =$$

$$= i\hbar\psi(p) + \cancel{i\hbar p\frac{d\psi(p)}{dp}} - \cancel{i\hbar p\frac{d\psi(p)}{dp}} =$$

$$= i\hbar\psi(p),$$

and of course $i\hbar\hat{1}|\psi\rangle \xrightarrow{\{|p\rangle\}} i\hbar\psi(p)$.

- Example: As a bit more of training, compute the commutator $[\hat{x}, \hat{p}^2]$ first abstractly, using $[\hat{x}, \hat{p}] = i\hbar\hat{1}$, then in both the above representations.

To compute $[\hat{x}, \hat{p}^2]$, it's easiest to use a general formula:

$$\boxed{[\hat{A}, \hat{B}\hat{C}] = \hat{B}[\hat{A}, \hat{C}] + [\hat{A}, \hat{B}]\hat{C}}$$

(prove it!), which yields:

$$\boxed{[\hat{x}, \hat{p}^2]} = \hat{p}[\hat{x}, \hat{p}] + [\hat{x}, \hat{p}]\hat{p} = \boxed{2i\hbar\hat{p}.}$$

Now in the position representation, $\hat{x} \xrightarrow{\{|x\rangle\}} x$ and $\hat{p}^2 \xrightarrow{\{|p\rangle\}} \left(-i\hbar\frac{d}{dx}\right)\left(-i\hbar\frac{d}{dx}\right) = -\hbar^2\frac{d^2}{dx^2}$ (second derivative; the minus sign is there because $(-i)^2 = -1$), and therefore for arbitrary $|\psi\rangle$:

$$[\hat{x}, \hat{p}^2]|\psi\rangle \xrightarrow{\{|x\rangle\}} x\left(-\hbar^2\frac{d^2}{dx^2}\right)\psi(x) - \left(-\hbar^2\frac{d^2}{dx^2}\right)x\,\psi(x) =$$

$$= -\hbar^2 x\frac{d^2\psi(x)}{dx^2} + \hbar^2\frac{d^2(x\psi(x))}{dx^2} =$$

$$= \left\{ \begin{aligned} &\frac{d(x\psi(x))}{dx} = \psi(x) + x\frac{d\psi(x)}{dx} \\ &\downarrow \\ &\frac{d^2(x\psi(x))}{dx^2} = \frac{d\psi(x)}{dx} + \frac{d}{dx}\left(x\frac{d\psi(x)}{dx}\right) = \frac{d\psi(x)}{dx} + \frac{d\psi(x)}{dx} + x\frac{d^2\psi(x)}{dx^2} = \\ &= 2\frac{d\psi(x)}{dx} + x\frac{d^2\psi(x)}{dx^2} \end{aligned} \right\} =$$

$$= \cancel{-\hbar^2 x\frac{d^2\psi(x)}{dx^2}} + 2\hbar^2\frac{d\psi(x)}{dx} + \cancel{\hbar^2 x\frac{d^2\psi(x)}{dx^2}} =$$

$$= 2\hbar^2\frac{d}{dx}\psi(x),$$

and there is: $2i\hbar\hat{p}|\psi\rangle \xrightarrow{\{|x\rangle\}} 2i\hbar\left(-i\hbar\frac{d}{dx}\right)\psi(x) = 2\hbar^2\frac{d}{dx}\psi(x)$, i.e. agreement.

Similarly in the momentum representation, $\hat{x} \xrightarrow{\{|p\rangle\}} i\hbar\frac{d}{dp}$ and $\hat{p}^2 \xrightarrow{\{|p\rangle\}} p^2$, and so for arbitrary $|\psi\rangle$:

$$[\hat{x}, \hat{p}^2]|\psi\rangle \xrightarrow{\{|p\rangle\}} \left(i\hbar\frac{d}{dp}\right)p^2\psi(p) - p^2\left(i\hbar\frac{d}{dp}\right)\psi(p) =$$

$$= i\hbar\frac{d(p^2\psi(p))}{dp} - i\hbar p^2\frac{d\psi(p)}{dp} =$$

$$= 2i\hbar p\,\psi(p) + \cancel{i\hbar p^2\frac{d\psi(p)}{dp}} - \cancel{i\hbar p^2\frac{d\psi(p)}{dp}} =$$

$$= 2i\hbar p\,\psi(p),$$

and there is: $2i\hbar\hat{p}|\psi\rangle \xrightarrow{\{|p\rangle\}} 2i\hbar p\,\psi(p)$, i.e. the same.

Let's summarize the results of the above two examples: The operator $[\hat{x}, \hat{p}] = i\hbar\hat{1}$ has the following position and momentum representations (in the sense of operators in the spaces of position/momentum wavefunctions, not in the sense of functions of two variables):

$$\boxed{\begin{aligned} &[\hat{x}, \hat{p}] \xrightarrow{\{|x\rangle\}} i\hbar, \\ &[\hat{x}, \hat{p}] \xrightarrow{\{|p\rangle\}} i\hbar. \end{aligned}}$$

The operator $[\hat{x}, \hat{p}^2] = 2i\hbar\hat{p}$ has the following position and momentum representations:

$$\boxed{\begin{array}{l} [\hat{x}, \hat{p}^2] \xrightarrow{\{|x\rangle\}} 2\hbar^2 \frac{d}{dx}, \\ [\hat{x}, \hat{p}^2] \xrightarrow{\{|p\rangle\}} 2i\hbar p. \end{array}}$$

• Example: We've discussed above that <u>formally speaking</u> the position and momentum representations of $\hat{x}$ are functions of two variables, $\langle x|\hat{x}|x'\rangle = x'\delta(x-x')$ and $\langle p|\hat{x}|p'\rangle = -i\hbar\frac{d(\delta(p'-p))}{dp'}$, but <u>practically speaking</u> they're operators in the spaces of the appropriate wavefunctions, $\hat{x} \xrightarrow{\{|x\rangle\}} x$, $\hat{x} \xrightarrow{\{|p\rangle\}} i\hbar\frac{d}{dp}$. Now let's see how this understanding can be applied to a computation of the inner product $\langle\psi|\hat{x}|\phi\rangle$ for two arbitrary kets $|\psi\rangle$ and $|\phi\rangle$.

<u>Formally</u>, to compute $\langle\psi|\hat{x}|\phi\rangle$ using the position representation, we insert two identities:

$$\langle\psi|\hat{x}|\phi\rangle = \int_{-\infty}^{+\infty}dx\int_{-\infty}^{+\infty}dx'\, \underbrace{\overbrace{\langle\psi|x\rangle}^{\text{BRA}}}_{\substack{\text{NUMBER}\\ \| \\ \psi(x)^*}}\underbrace{\overbrace{\langle x|\hat{x}|x'\rangle}^{\text{OPERATOR OPER. OPERATOR}}}_{\substack{\text{NUMBER}\\ \| \\ x'\delta(x-x')}}\underbrace{\overbrace{\langle x'|\phi\rangle}^{\text{KET}}}_{\substack{\text{NUMBER}\\ \| \\ \phi(x)}} =$$

$$\hat{1} = \int_{-\infty}^{+\infty}dx'|x'\rangle\langle x'|$$

$$\hat{1} = \int_{-\infty}^{+\infty}dx\,|x\rangle\langle x|$$

$$= \int_{-\infty}^{+\infty}dx\int_{-\infty}^{+\infty}dx'\,\psi(x)^*\,x'\,\delta(x-x')\,\phi(x) =$$

$$= \int_{-\infty}^{+\infty}dx\,\psi(x)^*\,x\,\phi(x).$$

To compute the same quantity using the momentum representation, we proceed analogously:

$$\langle\psi|\hat{p}|\phi\rangle = \int_{-\infty}^{+\infty}dp\int_{-\infty}^{+\infty}dp'\, \underbrace{\overbrace{\langle\psi|p\rangle}^{\text{BRA}}}_{\substack{\text{NUMBER}\\ \| \\ \psi(p)^*}}\underbrace{\overbrace{\langle p|\hat{x}|p'\rangle}^{\text{OPERATOR OPER. OPERATOR}}}_{\substack{\text{NUMBER}\\ \| \\ -i\hbar\frac{d(\delta(p'-p))}{dp'}}}\underbrace{\overbrace{\langle p'|\phi\rangle}^{\text{KET}}}_{\substack{\text{NUMBER}\\ \| \\ \phi(p')}} =$$

$$= \int_{-\infty}^{+\infty}dp\int_{-\infty}^{+\infty}dp'\,\psi(p)^*\,(-i\hbar)\frac{d(\delta(p'-p))}{dp'}\,\phi(p') = \ldots$$

Again, we encounter derivative of Dirac delta; you remember that the way to handle it, is to integrate by parts:

$$\dots = \int_{-\infty}^{+\infty} dp \int_{-\infty}^{+\infty} dp' \, \psi(p)^* (+i\hbar) \, \delta(p'-p) \frac{d\phi(p')}{dp'} =$$

(CHANGE OF SIGN DUE TO INTEGRATION BY PARTS)

$$= \int_{-\infty}^{+\infty} dp \, \psi(p)^* \, i\hbar \frac{d}{dp} \phi(p).$$

Hence we've derived that:

$$\boxed{\langle\psi|\hat{x}|\phi\rangle = \int_{-\infty}^{+\infty} dx \, \psi(x)^* x \, \phi(x) = \int_{-\infty}^{+\infty} dp \, \psi(p)^* \, i\hbar \frac{d}{dp} \phi(p),}$$

for any two kets $|\psi\rangle$ and $|\phi\rangle$.

But this calculation can be avoided if we notice that:

$$\boxed{\begin{array}{ll} |\phi\rangle \xrightarrow{\{|x\rangle\}} \phi(x), & \langle\psi| \xrightarrow{\{|x\rangle\}} \psi(x)^*, \\ |\phi\rangle \xrightarrow{\{|p\rangle\}} \phi(p), & \langle\psi| \xrightarrow{\{|p\rangle\}} \psi(p)^*, \end{array}}$$

and use the representation of $\hat{x}$ in the form of the differential operators x and $i\hbar\frac{d}{dp}$, as can be seen from the final formula.

To practice this simplification, consider the inner product $\langle\psi|\hat{p}|\phi\rangle$ for any two kets $|\psi\rangle$ and $|\phi\rangle$. You can compute it in the formal way (by insertion of two identities and so on), but you can equally well use the practical prescription, which <u>immediately</u> yields:

$$\boxed{\langle\psi|\hat{p}|\phi\rangle = \int_{-\infty}^{+\infty} dx \, \psi(x)^* (-i\hbar) \frac{d}{dx} \phi(x) = \int_{-\infty}^{+\infty} dp \, \psi(p)^* p \, \phi(p).}$$

This is the same as using the formulas from p. 23, $\langle x|\hat{p}|\phi\rangle = -i\hbar\frac{d}{dx}\phi(x)$, $\langle p|\hat{p}|\phi\rangle = p\psi(p)$, and inserting just one identity:

$$\langle\psi|\hat{p}|\phi\rangle = \int_{-\infty}^{+\infty} dx \, \langle\psi|x\rangle\langle x|\hat{p}|\phi\rangle = \int_{-\infty}^{+\infty} dx \, \psi(x)^* \left(-i\hbar\frac{d}{dx}\right) \phi(x),$$

$$\hat{1} = \int_{-\infty}^{+\infty} dx |x\rangle\langle x|$$

or:

$$\langle\psi|\hat{p}|\phi\rangle = \int_{-\infty}^{+\infty} dp \langle\psi|p\rangle\langle p|\hat{p}|\phi\rangle = \int_{-\infty}^{+\infty} dp\, \psi(p)^* p\, \phi(p).$$

$$\hat{1} = \int_{-\infty}^{+\infty} dp |p\rangle\langle p|$$

- Example: Warm-Up Problem 4.1. This exercise allows you to practice further what we've learned in the previous example. Here we've given a ket $|\psi\rangle$ which has the position representation $\psi(x) = \frac{1}{\sqrt[4]{\pi}\sqrt{s}} e^{-x^2/2s^2}$, where $s>0$, and we want to compute the inner products $\langle\psi|\hat{p}|\psi\rangle$ and $\langle\psi|\hat{p}^2|\psi\rangle$.

The first of these products reads:

$$\langle\psi|\hat{p}|\psi\rangle = \int_{-\infty}^{+\infty} dx\, \psi(x)^* (-i\hbar) \frac{d\psi(x)}{dx} =$$

$$= -i\hbar \int_{-\infty}^{+\infty} dx \frac{1}{\sqrt[4]{\pi}\sqrt{s}} e^{-\frac{x^2}{2s^2}} \frac{1}{\sqrt[4]{\pi}\sqrt{s}} e^{-\frac{x^2}{2s^2}} \left(-\frac{x}{s^2}\right) =$$

$$= \frac{i\hbar}{\sqrt{\pi}\, s^3} \int_{-\infty}^{+\infty} dx\, x\, e^{-\frac{x^2}{s^2}} = 0.$$

The reason we could so quickly tell that the result is 0, is another widely-used trick: notice that if a function $f(x)$ is odd, i.e. if $f(-x) = -f(x)$ for all x, then $\int_{-\infty}^{+\infty} dx\, f(x) = 0$. Proof is very simple:

$$\int_{-\infty}^{+\infty} dx\, f(x) = \int_0^{+\infty} dx\, f(x) + \int_{-\infty}^{0} dx\, f(x) = \int_0^{+\infty} dx\, f(x) + \int_0^{+\infty} dx\, f(-x) =$$

$$= \int_0^{+\infty} dx \left(f(x) + f(-x)\right) = 0.$$

In our case, $f(x) = x e^{-x^2/s^2}$, which is clearly odd: $f(-x) = -x e^{-(-x)^2/s^2} = -f(x)$.

The second of the products to compute is:

$$\langle\psi|\hat{p}^2|\psi\rangle = \int_{-\infty}^{+\infty} dx\, \psi(x)^* (-\hbar^2) \frac{d^2\psi(x)}{dx^2} =$$

$$= -\hbar^2 \int_{-\infty}^{+\infty} dx \frac{1}{\sqrt[4]{\pi}\sqrt{s}} e^{-\frac{x^2}{2s^2}} \frac{1}{\sqrt[4]{\pi}\sqrt{s}} e^{-\frac{x^2}{2s^2}} \frac{1}{s^2}\left(\frac{x^2}{s^2} - 1\right) =$$

$$= \frac{\hbar^2}{\sqrt{\pi}\, s^3} \int_{-\infty}^{+\infty} dx\, e^{-\frac{x^2}{s^2}} \left(1 - \frac{x^2}{s^2}\right) = \ldots$$

To find this integral, first notice that if a function $f(x)$ is even, i.e. if $f(-x)=f(x)$, then $\int_{-\infty}^{+\infty} dx\, f(x) = 2\int_0^{+\infty} dx\, f(x)$. Here $f(x) = e^{-x^2/s^2}\left(1-\frac{x^2}{s^2}\right)$, which is clearly even, so:

$$\ldots = \frac{2\hbar^2}{\sqrt{\pi}\, s^3}\int_0^{+\infty} dx\, e^{-\frac{x^2}{s^2}}\left(1-\frac{x^2}{s^2}\right) = \ldots$$

These integrals are known as the Gaussian integrals, and are among the most important integrals in physics, so it's good you learn about them:

$$\boxed{\begin{aligned} \int_0^{+\infty} dx\, e^{-\frac{x^2}{s^2}} &= \frac{\sqrt{\pi}\, s}{2}, \\ \int_0^{+\infty} dx\, \frac{x^2}{s^2} e^{-\frac{x^2}{s^2}} &= \frac{\sqrt{\pi}\, s}{4} \end{aligned}}$$

(more generally, you can find a formula for $\int_0^{+\infty} dx\, \frac{x^{2n}}{s^{2n}} e^{-x^2/s^2}$). This leads to:

$$\ldots = \frac{2\hbar^2}{\sqrt{\pi}\, s^3}\left(\frac{\sqrt{\pi}\, s}{2} - \frac{\sqrt{\pi}\, s}{4}\right) = \frac{\cancel{2}\hbar^2}{\cancel{\sqrt{\pi}}\, s^{\cancel{3}2}}\, \frac{\cancel{\sqrt{\pi}}\, \cancel{s}}{\cancel{4}_2} = \frac{\hbar^2}{2s^2}.$$

We've thus found that for the ket $|\psi\rangle$ which has the position representation $\psi(x) = \frac{1}{\sqrt[4]{\pi}\sqrt{s}} e^{-x^2/2s^2}$, $\langle\psi|\hat{p}|\psi\rangle = 0$, $\langle\psi|\hat{p}^2|\psi\rangle = \hbar^2/2s^2$. You can practice this further by showing that for this particular ket, $\langle\psi|\hat{x}|\psi\rangle = 0$, $\langle\psi|\hat{x}^2|\psi\rangle = s^2/2$. Check also that this ket is normalized, i.e. that $\langle\psi|\psi\rangle = 1$.

(As an exercise in the trick from p. 19 of "bringing down from an exponent", you can derive the second Gaussian integral from the first one: you will need to "bring down" x^2 from e^{-x^2/s^2}, which requires $d/d(-1/s^2)$. Derive in this way the general $\int_0^{+\infty} dx\, x^{2n} e^{-x^2/s^2}$, for $n=1,2,3,\ldots$ Remember this, because you'll encounter this kind of calculation quite often in physics, for example in statistical mechanics or quantum field theory. The result reads:

$$\boxed{\int_0^{+\infty} dx\, \frac{x^{2n}}{s^{2n}} e^{-x^2/s^2} = \frac{\sqrt{\pi}}{2^{2n}}\frac{(2n-1)!}{(n-1)!}\, s.}$$

(Do you see why $\frac{1}{s}\int_0^{+\infty} dx\, \frac{x^{2n}}{s^{2n}} e^{-x^2/s^2}$ is independent of s?))

SUMMARY

- The basic objects in Dirac notation:
  - (1) $\boxed{|\alpha\rangle,}$ ket, a vector.
  - (2) $\boxed{\langle\alpha|,}$ bra, a vector.
  - (3) $\boxed{\langle\alpha|\beta\rangle,}$ inner product, a complex number.
  - (4) $\boxed{|\alpha\rangle\langle\beta|,}$ outer product, a linear operator.

- Defining properties of inner product:

(1)
$$\boxed{\begin{aligned}&\langle a\alpha+b\beta|\gamma\rangle = a^*\langle\alpha|\gamma\rangle + b^*\langle\beta|\gamma\rangle, \quad a,b\in\mathbb{C},\\ &\langle\gamma|a\alpha+b\beta\rangle = a\langle\gamma|\alpha\rangle + b\langle\gamma|\beta\rangle, \quad a,b\in\mathbb{C}\end{aligned}}$$

(antilinearity in the first argument, linearity in the second argument).

(2)
$$\boxed{\begin{aligned}&\langle\alpha|\alpha\rangle\in\mathbb{R}_{\geq 0}, \quad \text{for all } |\alpha\rangle,\\ &\langle\alpha|\alpha\rangle = 0 \Rightarrow |\alpha\rangle = 0.\end{aligned}}$$

They yield the following properties:

(1)
$$\boxed{\langle\alpha|\beta\rangle^* = \langle\beta|\alpha\rangle, \quad \text{for all } |\alpha\rangle, |\beta\rangle.}$$

(2)
$$\boxed{\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle \geq |\langle\alpha|\beta\rangle|^2, \quad \text{for all } |\alpha\rangle, |\beta\rangle}$$

(Cauchy-Schwarz inequality).

- The basic reasons for the use of Dirac notation:
  - (1) "Different viewpoints", for example:

$$\boxed{\overbrace{\langle\alpha|}^{\text{BRA}}\overbrace{\beta\rangle\langle\gamma|}^{\text{OPERATOR}}\overbrace{\hat{A}}^{\text{OPER.}}\overbrace{|\delta\rangle\langle\epsilon|}^{\text{OPERATOR}}\overbrace{\zeta\rangle}^{\text{KET}}} \leftarrow \text{"OLD VIEWPOINT"}$$

$$\boxed{\underbrace{\langle\alpha|\beta\rangle}_{\text{NUMBER}}\underbrace{\langle\gamma|\hat{A}|\delta\rangle}_{\text{NUMBER}}\underbrace{\langle\epsilon|\zeta\rangle}_{\text{NUMBER}}.} \leftarrow \text{"NEW VIEWPOINT"}$$

  - (2) Kets/bras are easy to describe (get used to new ways of describing vectors!), e.g.:

$$\boxed{|\text{living Schrödinger's cat}\rangle, \quad |\uparrow\rangle, \quad |+\rangle, \quad |j,l,m\rangle, \quad \text{etc.}}$$

(3) The completeness relation (decomposition of identity): For any orthonormal basis $\{|i\rangle : i = 1, 2, \ldots, N\}$ (discrete case) / $\{|x\rangle : x \in \mathbb{R}\}$ (continuous case):

$$\boxed{\sum_{i=1}^{N} |i\rangle\langle i| = \hat{1},}$$

$$\boxed{\int_{-\infty}^{+\infty} dx\, |x\rangle\langle x| = \hat{1}.}$$

"Insertion of identity" is one of the basic techniques in calculations in Dirac notation, greatly simplifying them.

- Two types of bases we use:

(1) Discrete bases:

$$\boxed{\{|i\rangle : i = 1, 2, \ldots, N\},}$$

where N can be finite or $N = +\infty$.

(2) Continuous bases:

$$\boxed{\{|x\rangle : x \in \mathbb{R}\}.}$$

All the calculations are completely analogous in these two cases provided:

(1) We exchange all sums with integrals.

(2) We exchange all Kronecker deltas δ_{ij} with Dirac deltas $\delta(x - x')$.

The basic property of Kronecker / Dirac delta is:

(1) $$\boxed{\sum_i f_i \delta_{ij} = f_j.}$$

(2) $$\boxed{\int_{-\infty}^{+\infty} dx\, f(x)\, \delta(x - x') = f(x').}$$

(Actually, the integration doesn't need to be from $-\infty$ to $+\infty$; it's enough it includes the point x', i.e. $\int_a^b dx\, f(x)\, \delta(x - x') = f(x')$ if $x' \in (a, b)$. Otherwise, i.e. if $x' \notin (a, b)$, the result is 0.)

The bases we consider will always be orthonormal:

(1) $$\boxed{\langle i|j\rangle = \delta_{ij}, \quad \text{for all } i,j = 1,2,\dots,N.}$$

(2) $$\boxed{\langle x|x'\rangle = \delta(x-x'), \quad \text{for all } x, x' \in \mathbb{R}.}$$

- Representation of a ket $|\psi\rangle$ in such an orthonormal basis is:

$$\boxed{|\psi\rangle = \sum_{i=1}^{N} |i\rangle \psi_i, \quad \psi_i = \langle i|\psi\rangle,}$$

$$\boxed{|\psi\rangle = \int_{-\infty}^{+\infty} dx\, |x\rangle \psi(x), \quad \psi(x) = \langle x|\psi\rangle,}$$

i.e. it's a column of N complex numbers $[\psi] \equiv \begin{pmatrix} \psi_1 \\ \vdots \\ \psi_N \end{pmatrix}$ (discrete case) / a complex function of one variable $\psi(x)$ (continuous case). Obtained by: $\underset{1}{\uparrow}|\psi\rangle$.

- Representation of an operator $\hat{A}$ in such an orthonormal basis is:

$$\boxed{\hat{A} = \sum_{i=1}^{N}\sum_{j=1}^{N} |i\rangle\langle j| A_{ij}, \quad A_{ij} = \langle i|\hat{A}|j\rangle,}$$

$$\boxed{\hat{A} = \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dx'\, |x\rangle\langle x'|\, A(x,x'), \quad A(x,x') = \langle x|\hat{A}|x'\rangle,}$$

i.e. it's a complex $N \times N$ matrix $[A] \equiv \begin{pmatrix} A_{11} & \cdots & A_{1N} \\ \vdots & \ddots & \vdots \\ A_{N1} & \cdots & A_{NN} \end{pmatrix}$ (discrete case) / a complex function of two variables $A(x,x')$ (continuous case). Obtained by: $\underset{1}{\uparrow}\hat{A}\underset{1}{\uparrow}$.

- To gain practice in using representations we can rewrite some abstract expressions in a given representation, for example:

(1) $$\boxed{\langle \psi|\phi\rangle = \sum_{i=1}^{N} \psi_i^* \phi_i = [\psi]^\dagger[\phi],}$$

$$\boxed{\langle \psi|\phi\rangle = \int_{-\infty}^{+\infty} dx\, \psi(x)^* \phi(x).}$$

In particular:

$$\boxed{\langle \psi|\psi\rangle = \sum_{i=1}^{N} |\psi_i|^2 = [\psi]^\dagger[\psi],}$$

$$\boxed{\langle \psi|\psi\rangle = \int_{-\infty}^{+\infty} dx\, |\psi(x)|^2.}$$

(2) $$\boxed{\langle\psi|\hat{A}|\phi\rangle = \sum_{i=1}^{N}\sum_{j=1}^{N}\psi_i^* A_{ij}\,\phi_j = [\psi]^\dagger[A][\phi],}$$

$$\boxed{\langle\psi|\hat{A}|\phi\rangle = \int_{-\infty}^{+\infty}dx\int_{-\infty}^{+\infty}dx'\;\psi(x)^* A(x,x')\,\phi(x').}$$

(3) The equation $\hat{A}|\psi\rangle = |\phi\rangle$ can be rewritten as:

$$\boxed{\sum_{j=1}^{N} A_{ij}\,\psi_j = \phi_i, \quad \text{i.e.} \quad [A][\psi] = [\phi],}$$

$$\boxed{\int_{-\infty}^{+\infty}dx'\,A(x,x')\,\psi(x') = \phi(x).}$$

• <u>Change of representation of a ket $|\psi\rangle$</u> is:

$$\boxed{\tilde{\psi}_i = \sum_{j=1}^{N} U_{ij}\,\psi_j, \quad \text{i.e.} \quad [\tilde{\psi}] = [U][\psi], \qquad U_{ij} = \langle\tilde{i}|j\rangle,}$$

$$\boxed{\tilde{\psi}(x) = \int_{-\infty}^{+\infty}dx'\,U(x,x')\,\psi(x'), \qquad U(x,x') = \langle\tilde{x}|x'\rangle,}$$

where we move from the <u>"old basis"</u> $\{|i\rangle : i = 1,2,\dots,N\}$ (discrete case) / $\{|x\rangle : x\in\mathbb{R}\}$ (continuous case) to the <u>"new basis"</u> $\{|\tilde{i}\rangle : i = 1,2,\dots,N\}$ (discrete case) / $\{|\tilde{x}\rangle : x\in\mathbb{R}\}$ (continuous case).

The <u>transition matrix</u> $[U]$ / $U(x,x')$ is <u>unitary</u>.

You don't neccessarily need to remember this formula if you remember how to quickly derive it – <u>by "insertion of identity": $\langle\tilde{i}\underset{\stackrel{\uparrow}{\hat{1}}}{|}\psi\rangle$.</u>

• <u>Change of representation of an operator $\hat{A}$</u> is:

$$\boxed{\tilde{A}_{ij} = \sum_{k=1}^{N}\sum_{l=1}^{N}\underbrace{U_{ik}}_{=\langle\tilde{i}|k\rangle} A_{kl}\underbrace{U^*_{jl}}_{=\langle l|\tilde{j}\rangle}, \qquad \text{i.e.} \qquad [\tilde{A}] = [U][A][U]^\dagger,}$$

$$\boxed{\tilde{A}(x,x') = \int_{-\infty}^{+\infty}dx''\int_{-\infty}^{+\infty}dx'''\;\underbrace{U(x,x'')}_{=\langle\tilde{x}|x''\rangle}A(x'',x''')\underbrace{U(x',x''')^*}_{=\langle x'''|\tilde{x}'\rangle}.}$$

Again, it's enough you're sure how to quickly derive them – <u>by "insertion of identity" twice: $\langle\tilde{i}\underset{\stackrel{\uparrow}{\hat{1}}}{|}\hat{A}\underset{\stackrel{\uparrow}{\hat{1}}}{|}\tilde{j}\rangle$.</u>

- We've introduced two very important continuous bases in QM: <u>the position basis</u> and <u>the momentum basis</u>:

$$\boxed{\begin{aligned}&\{|x\rangle : x\in\mathbb{R}\},\\ &\{|p\rangle : p\in\mathbb{R}\}.\end{aligned}}$$

The transition "matrix" between them is:

$$\boxed{U(p,x) = \langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}}\, e^{-\frac{i}{\hbar}px}\,;}$$

it's unitary:

$$\boxed{\frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} dp\, e^{\frac{i}{\hbar}p(x-x')} = \delta(x-x').}$$

The representations of a ket $|\psi\rangle$ in these bases, $\psi(x)$ and $\psi(p)$, are called <u>the position and momentum wavefunctions</u>:

$$\boxed{\begin{aligned}&|\psi\rangle = \int_{-\infty}^{+\infty} dx\, |x\rangle\, \psi(x), &&\psi(x) = \langle x|\psi\rangle,\\ &|\psi\rangle = \int_{-\infty}^{+\infty} dp\, |p\rangle\, \psi(p), &&\psi(p) = \langle p|\psi\rangle.\end{aligned}}$$

They're related by <u>the Fourier transformation</u>:

$$\boxed{\begin{aligned}&\psi(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty} dx\, e^{-\frac{i}{\hbar}px}\,\psi(x),\\ &\psi(x) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty} dp\, e^{+\frac{i}{\hbar}px}\,\psi(p).\end{aligned}}$$

You can write similar relations between the representations of an operator $\hat{A}$ in these bases, $A(x,x') = \langle x|\hat{A}|x'\rangle$ and $A(p,p') = \langle p|\hat{A}|p'\rangle$.

- We've introduced also two very important operators in QM: <u>the position operator $\hat{x}$</u> and <u>the momentum operator $\hat{p}$</u>.

<u>Their representations</u> in the position and momentum bases are:

$$\boxed{\begin{aligned}&\langle x|\hat{x}|x'\rangle = x'\,\delta(x-x'),\\ &\langle p|\hat{x}|p'\rangle = -i\hbar\,\frac{d(\delta(p'-p))}{dp'},\end{aligned}}$$

$$\boxed{\begin{aligned}\langle x|\hat{p}|x'\rangle &= +i\hbar\frac{d(\delta(x'-x))}{dx'},\\ \langle p|\hat{p}|p'\rangle &= p'\delta(p-p').\end{aligned}}$$

More practically:

$$\boxed{\begin{aligned}\langle x|\hat{x}|\psi\rangle &= x\psi(x),\\ \langle p|\hat{x}|\psi\rangle &= +i\hbar\frac{d\psi(p)}{dp},\end{aligned}}$$

$$\boxed{\begin{aligned}\langle x|\hat{p}|\psi\rangle &= -i\hbar\frac{d\psi(x)}{dx},\\ \langle p|\hat{p}|\psi\rangle &= p\psi(p),\end{aligned}}$$

which amounts for calling "the representations of $\hat{x}$ and $\hat{p}$ in the position and momentum bases" the following differential operators (acting in the spaces of the appropriate wavefunctions):

$$\boxed{\begin{aligned}&\hat{x} \xrightarrow{\{|x\rangle\}} x,\\ &\hat{x} \xrightarrow{\{|p\rangle\}} +i\hbar\frac{d}{dp},\end{aligned}}$$

$$\boxed{\begin{aligned}&\hat{p} \xrightarrow{\{|x\rangle\}} -i\hbar\frac{d}{dx},\\ &\hat{p} \xrightarrow{\{|p\rangle\}} p\ ;\end{aligned}}$$

this understanding shortens calculations featuring $\hat{x}$ or $\hat{p}$.

- In the course of derivation of the above formulae, we've encountered a few useful tricks:

  (1) "Bringing down from an exponent": Integrals like $\int_{-\infty}^{+\infty}dx\, x\, e^{\frac{i}{\hbar}x(p'-p)}$ can be computed by noticing that $\boxed{\frac{d}{dp'}\left(e^{\frac{i}{\hbar}x(p'-p)}\right) = \frac{i}{\hbar}x\, e^{\frac{i}{\hbar}x(p'-p)}}$ (if you have another power of x, e.g. x^2, you use more derivatives), and remembering that $\boxed{\frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty}dx\, e^{\frac{i}{\hbar}x(p'-p)} = \delta(p'-p)}$ (see above p. 34). Many similar integrals are computed in this way (see e.g. p. 29). This trick is also called "differentiation under integration" or "differentiation over a parameter", and is very useful in physics.

(2) In QM you often integrate by parts:

$$\boxed{\int dy \frac{df(y)}{dy} g(y) = f(y)g(y) - \int dy\, f(y) \frac{dg(y)}{dy}.}$$

When your integrals have limits at infinity, usually the term $f(y)g(y)\big|_{y=-\infty}^{y=+\infty}$ will vanish, because all the wavefunctions in QM must vanish at infinity; then simply:

$$\boxed{\int_{-\infty}^{+\infty} dy \frac{df(y)}{dy} g(y) = -\int_{-\infty}^{+\infty} dy\, f(y) \frac{dg(y)}{dy}.}$$

(3) Derivative of Dirac delta is understood by integration by parts:

$$\boxed{\int_{-\infty}^{+\infty} dx\, f(x) \frac{d(\delta(x-x'))}{dx} = -\int_{-\infty}^{+\infty} dx \frac{df(x)}{dx} \delta(x-x') = -\frac{df(x')}{dx'}.}$$

(4) When you compute commutators, the following formula is useful:

$$\boxed{[\hat{A}, \hat{B}\hat{C}] = \hat{B}[\hat{A}, \hat{C}] + [\hat{A}, \hat{B}]\hat{C}.}$$

(5) $f(x)$ is odd, i.e. $f(-x) = -f(x)$ for all x $\Rightarrow$ $\int_{-\infty}^{+\infty} dx\, f(x) = 0$,

$f(x)$ is even, i.e. $f(-x) = +f(x)$ for all x $\Rightarrow$ $\int_{-\infty}^{+\infty} dx\, f(x) = 2\int_{0}^{+\infty} dx\, f(x)$.

(6) The two lowest Gaussian integrals (one of the most important integrals in physics) are:

$$\boxed{\begin{aligned} \int_{0}^{+\infty} \frac{dx}{s} e^{-x^2/s^2} &= \frac{\sqrt{\pi}}{2}, \\ \int_{0}^{+\infty} \frac{dx}{s} \frac{x^2}{s^2} e^{-x^2/s^2} &= \frac{\sqrt{\pi}}{4}, \end{aligned}}$$

for $s > 0$. Trick (1) is used to derive the second one, and the higher, from the first one, to get for $n = 1, 2, 3, \ldots$:

$$\boxed{\int_{0}^{+\infty} \frac{dx}{s} \frac{x^{2n}}{s^{2n}} e^{-x^2/s^2} = \frac{\sqrt{\pi}}{2^{2n}} \frac{(2n-1)!}{(n-1)!}.}$$

(And from trick (5) you know that these integrals from $-\infty$ to $+\infty$ will give twice the above results, e.g. $\int_{-\infty}^{+\infty} \frac{dx}{s} e^{-x^2/s^2} = \sqrt{\pi}$.)